A selection of nonequilibrium issues

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Abstract: We give a pedagogical introduction to a selection of recently discussed topics in nonequilibrium statistical mechanics, concentrating mostly on formal structures and on general principles. Part I contains an overview of the formalism of lattice gases that we use to explain various symmetries and inequalities generally valid for nonequilibrium systems, including the fluctuation symmetry, Jarzynski equality, and the direction of currents. In Part II we concentrate on the macroscopic state and how entropy provides a bridge between microscopic dynamics and macroscopic irreversibility; included is a construction of quantum macroscopic states and a result on the equivalence of ensembles.

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1. Introduction

A good way to learn about possible constructions of nonequilibrium statistical mechanics probably proceeds via the study of simple model systems. Traditionally, the so called stochastic lattice gases are playing there a prime role. A very early example is the Ehrenfest model. Not only was it important as one of the many urn models illustrating strategies and results from probability theory and from statistics, but it remains instrumental in learning about relaxation and about detailed balance, see e.g. [29] where Mark Kac does not seem to hesitate in calling the Ehrenfest model one of the most important models in all of physics. We will encounter that Ehrenfest model in the first section.

Over the last decades, many other lattice gas models have been invented. Often they appear attractive because they obey simple updating rules and they are rather easy to visualize and to simulate (at least today). Yet, their behavior is rich, including sometimes clear examples of emergent behavior. The latter refers to the organization of robust structures or patterns, of critical behavior, and of phase transitions, which result from some collective or cooperative behavior between the many interacting components. They have appeared in interdisciplinary contexts, varying from models of traffic, to models of turbulence or to models for the spreading of infections, in computer science, in economy etc. On the more mathematics side, we have here an interesting ground for exploring and extending the theory of spatially extended Markov processes. The role of the spatial architecture of the processes has recently been more in the center of attention, e.g. in discussions of processes on random graphs, small worlds etc. In recent versions, the architecture (or graph) also undergoes a dynamics, in interaction with the particles. Clearly these lattice gas models have proven their use already. A few books where mathematical and statistical mechanical introductions are found to the theory of lattice gases are [30, 36, 52].

Many good references link stochastic lattice gases with fundamental problems in physics, be it in the context of turbulence or in the derivation of hydrodynamic equations. In the present notes, we bring together a number of recent results in the construction of nonequilibrium statistical mechanics, as they appear for some simple stochastic lattice gas. The emphasis will be mostly on formal relations, from which both mathematical and physics treatments can find inspirations. We hope that this provides some step in a wider understanding of nonequilibrium issues in other and more realistic models. Indeed, one should

remain aware that stochastic lattice gases are often only effective tools. They are Markovian from the start and their transition rates depend on some *ad hoc* choices. They are stochastic and there is no specification of a larger environment.

After a short reminder of aspects of a Markov dynamics for one particle, we introduce the main models in Section 3. That is continued in Section 4 where the steady state is further specified. In all that we work with a finite one-dimensional system on which there is a particle hopping in the bulk of the system and a birth and death process at the two boundary sites. We consider a time-dependent version of the dynamics in Section 5. The main tool is provided by a Lagrangian set-up in which a Girsanov formula specifies the action (Section 6). Section 7 gives the main fluctuation relations in the form of a Jarzynski identity (relating the irreversible work with the change in free energy) and of a fluctuation symmetry in the particle current (a so called steady state fluctuation theorem). While the results are mainly well-known we are not aware of a similar *unifying* presentation in the literature. There remain however very many nonequilibrium issues which are not treated in these notes. Some remarks are devoted to them in the final section.

2. One walker

Consider the set $K = \{0, \ldots, N\}$ and the discrete time Markov chain with transition probabilities $p(x, x') = x/N$ if $x' = x - 1$ and $p(x, x') = 1 - x/N$ if $x' = x + 1$ for $x, x' \in K$. One interpretation is to think of the state $x \in K$ as the number of particles in one of two vessels. The total number of particles over the two vessels is fixed equal to N. At each discrete time moment, one of the N particles is randomly selected and moved to the other vessel from where it was. That model is known as the Ehrenfest model (or dog-flea model).
As a mathematical object we have here an irreducible (but not aperiodic!) Markov chain (x_n) that satisfies the condition of detailed balance with respect to the stationary measure

$$\rho(x) = 2^{-N} \frac{N!}{x!(N-x)!}, \qquad x \in K$$

That condition of detailed balance

$$p(x, x')\, \rho(x) = p(x', x)\, \rho(x')$$

expresses the time-reversibility of the stationary process. Indeed, let $\boldsymbol{P}_\rho$ denote the stationary process on $K^{\mathbb{Z}}$ and define $y_n = x_{-n}$. The process (y_n) is Markovian with stationary law ρ. Its law is denoted by $\boldsymbol{P}_\rho \Theta$ where Θ stands for time-reversal. We show that $\boldsymbol{P}_\rho \Theta = \boldsymbol{P}_\rho$ as a consequence of the condition of detailed balance. The basic observation

is that the transition probability for the process (y_n) is via Bayes' formula

$$q(y, y') = \text{Prob}[y_{n+1} = y' \mid y_n = y] = p(y', y) \frac{\rho(y')}{\rho(y)} = p(y, y')$$

Therefore, the condition of detailed balance is equivalent with the time-reversibility.

There is an easy way to generalize the above set-up. Let us first make the step to continuous time. We are now speaking about rates $c(x, y) \geq 0$ (or, transition probabilities per unit time) for the transition $x \to y$. If we assume that

$$c(x, y) = a(x, y)e^{[V(x)-V(y)]/2}$$

where $a(x, y) = a(y, x)$ is symmetric, then still

$$\frac{c(x, y)}{c(y, x)} = e^{[V(x)-V(y)]} \tag{2.1}$$

and $\rho(x) \propto \exp[-V(x)]$ is a reversible measure.

A new interpretation arises when thinking of the set $\{0, 1, \ldots, N\}$ as the sites of a lattice interval, with the usual nearest neighbor connections. The rates $c(x, y)$ could be taken non-zero only if $y = x \pm 1$ in which case we have a nearest neighbor walk. The condition of detailed balance (2.1) assures that the walker will not drift; there is a potential landscape $V(x)$, $x = 0, \ldots, N$ which could be periodically repeated to cover all of $\mathbb{Z}$ if wished.

There are ways to break detailed balance. One could for example insert a non-zero transition rate for moving between the states (sites) $0 \leftrightarrow N$, and then take $c(x, x + 1) = p$, $c(x, x - 1) = q \neq p$, $N + 1 = 0$. In that case, say with $p > q$ there is a drift that the particle moves more $x \to x + 1$ than $x \to x - 1$; there appears a net current.

More generally, we can think of parameterizing the rates via

$$c(x, y) = a(x, y)\, e^{[V(x)-V(y)]/2}\, e^{s(x,y)/2}$$

where $s(x, y) = -s(y, x)$ would be antisymmetric. It turns out that this term $s(x, y)$ has often an interesting physical interpretation. In what follows we will see it related to the entropy production. The entropy production is a physical notion that has arisen within irreversible thermodynamics, see e.g [21]. It goes well with considerations close to equilibrium. The influence of the time-symmetric factor $a(x, y)$ is less understood.

The following sections will study some of the aspects above for multi-particle models. We now have a (possibly variable) number of particles and they move on the lattice following certain hopping rules. The effect of having many particles can result in (simpler) hydrodynamic

behavior for macroscopic variables such as the density profile, but we will concentrate on the fluctuations instead.

3. Stochastic lattice gases

We start with a description of what is typically involved in stochastic lattice gases. We do not give the most general definitions but we specify to one special class.

3.1. **States.** By a lattice gas we understand a collection of particles whose positions are confined to the sites of a lattice. In some models the particles still have a momentum, most often with a finite number of possible values. Or, the particles can have extra decorations such as color or spin. Here we do not consider that.[4] The system thus consists of identical particles that can jump from site to site on the given architecture. The states of the system are assignments to each site of the number of particles. To be specific we consider the finite linear chain $\Lambda_N = \{-N, -N+1, \ldots, 0, 1, \ldots, N-1, N\}$. The endpoints $i = \pm N$ in Λ_N will play a special role in what follows; we call them the boundary of the system while the other sites are in the bulk. Two sites i, j are nearest neighbors when $j = i \pm 1$.
We allow at most one particle per site i. We say that site i can be vacant or occupied. The state space (or the configuration space) is the finite set $K = \{0,1\}^{\Lambda_N}$. Elements of K are denoted by $\eta, \eta', \xi, \ldots$ and we write $\eta(i) \in \{0,1\}$ for the occupation at site $i \in \Lambda_N$.

3.2. **Energy, entropy and particle number.** One imagines a function H typically referred to as the Hamiltonian of the system,[5] that measures the energy of the state η. There is a great freedom of choice and all depends on the context or on the specific purpose. It does not hurt however to suppose something specific, say an energy function consisting of two terms:

$$H(\eta) = -B \sum_{i=-N}^{N} \eta(i) - \kappa \sum_{i=-N}^{N-1} \eta(i)\,\eta(i+1), \qquad (3.1)$$

where B and κ are some constants. The first term contributes an energy $-B$ per particle being present in the system and the second term takes into account some form of nearest neighbor interaction related to

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[4] An important ingredient of the Hamiltonian (or symplectic) structure is thus lost. In particular the kinematical time-reversal that would normally change the sign of the velocities is absent.

[5] It is of course not a Hamiltonian in the strict sense of analytical mechanics. The word Hamiltonian refers here more to the quantum world where one considers for example the hopping of electrons in a crystal structure. A mathematically precise correspondence, also for the dynamical properties, can often be achieved via the so called weak coupling limit or within the framework of Fermi's Golden Rule.

the relative concentration of particles on neighboring sites.

Speaking of energy reminds us of its conservation law. We can indeed imagine that our system is in thermal contact with a very large heat bath at inverse temperature β (Boltzmann's constant is set equal to one), and for which all relevant changes are determined by the transitions in the system. In particular, every change $H(\eta') - H(\eta)$ in energy of the system is accompanied with the opposite change $\Delta E(\eta, \eta') = -(H(\eta') - H(\eta))$ of energy in the bath.[6] Imagining that the energy change of the reservoir is thermodynamically reversible, we associate to it a change of entropy in the reservoir equal to

$$\Delta S_{\text{res}} = \beta \Delta E(\eta, \eta') = -\beta(H(\eta') - H(\eta))$$

In other words, every change $\eta \to \eta'$ in the system's configuration entails an entropy flux, that is β times the heat dissipated in the thermal reservoir.[7]

For equilibrium purposes with just one heat bath, the relevant thermodynamic potential is the Helmholtz free energy. Its statistical mechanical version is

$$F = -\frac{1}{\beta} \log Z, \qquad Z = \sum_{\eta \in K} e^{-\beta H(\eta)}$$

Observe that if we change some parameter in H, e.g. the coupling coefficient κ in (3.1) (for fixed temperature), then the change in free energy $F = F(\kappa)$ equals the expected change in energy:

$$\frac{\mathrm{d}F}{\mathrm{d}\kappa} = \left\langle \frac{\mathrm{d}H}{\mathrm{d}\kappa} \right\rangle, \qquad H = H_\kappa$$

where

$$\langle g \rangle = \frac{1}{Z} \sum_{\eta \in K} g(\eta) \, e^{-\beta H(\eta)}$$

is the thermal expectation.

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[6] In a more microscopic set-up, including a description of the degrees of freedom in the heat bath, one would need to specify a more exact decomposition of the total energy into the system part and the part that belongs to the reservoir. There would also be interaction terms, the coupling, that contain both system and reservoir variables. Obviously, some convention is then needed of what is system and what is reservoir variable.

[7] On a scale where one supposes that the η give the full microscopic description of the system, there is no associated change of entropy in the system. The total change of entropy (also called, the entropy production) is then also equal to $-\beta(H(\eta') - H(\eta))$. Most of the time however, there is a further *lower* level of description of the system variables with an associated degeneracy.

Another important observable is the particle number. We write

$$\mathcal{N}_{[j,k]}(\eta) = \sum_{i=j}^{k} \eta(i)$$

for the total number of particles in the lattice interval $[j, k] \cap \Lambda_N$, $-N \leq j \leq k \leq N$. By construction, here we have that the particle numbers $\mathcal{N}_{[j,k]} \leq 2N + 1$ are *a priori* uniformly bounded. The total number of particles is denoted by $\mathcal{N} = \mathcal{N}_{[-N,N]}$.

Making the correspondence with a gas again makes us think of a conservation law, now of the total number of particles. In what follows, we imagine that the system is also in contact with a particle reservoir at its boundary. Through the endpoints $i = \pm N$ particles can enter or leave the system. We can also speak of a birth or a death of a particle at these sites. In Section 4.2 we will introduce the particle currents. As particles can carry energy (see e.g. the first term in (3.1)), the flow of particles in and out of the system can also contribute to the change of energy in the reservoir, and hence to changes in entropy.

The equilibrium ensemble that allows both the exchange of energy and of particles is the grand-canonical one. It gives probabilities

$$\mathbb{P}^{\beta,a}[\eta] = \frac{1}{\mathcal{Z}} e^{a \sum \eta(i)} e^{-\beta H(\eta)} \tag{3.2}$$

where $\mathcal{Z} = \mathcal{Z}(a, \beta, N)$ is a normalization factor. The constant a is called the chemical potential and in equilibrium it refers to and it is determined by the concentration of particles in the (imagined very large) environment.

3.3. **Dynamics.** The dynamics is given by a continuous time Markov process on K. We distinguish two modes of updating:

- A particle can jump (or hop) to nearest neighbor sites. That is a diffusion mechanism. We will not add external fields to the dynamics not to impose a bulk drift or bias;
- Particles can leave or enter the system at the boundary. That is a reaction mechanism. The system will be boundary driven.

We introduce some further notation to formalize the dynamics. As we only consider symmetric hopping, it is useful to introduce the transformation

$$\eta^{i,j}(k) = \begin{cases} \eta(k) & \text{if } k \neq i,\, k \neq j; \\ \eta(i) & \text{if } k = j; \\ \eta(j) & \text{if } k = i \end{cases} \tag{3.3}$$

That defines the configuration obtained from η after switching the occupation of the sites i, j. We allow only the hopping of particles to neighboring sites $j = i \pm 1$. The rate of the transition due to that

diffusion mechanism is taken as

$$C(i, j, \eta) = \exp\left[-\frac{\beta}{2}(H(\eta^{i,j}) - H(\eta))\right], \quad |i - j| = 1 \qquad (3.4)$$

where $H(\eta^{i,j})$ is the energy function after the transition and $H(\eta)$ is that corresponding to the initial configuration.

Analogously, we define the rate of birth and death $\eta \to \eta^i$ of the particles as

$$C(i, \eta) = e^{-a_i \eta(i)} \exp\left[-\frac{\beta}{2}(H(\eta^i) - H(\eta))\right] \qquad (3.5)$$

where $H(\eta^i)$ is the energy function after the transition to η^i, the new configuration after the birth or the death of a particle at site i:

$$\eta^i(k) = \begin{cases} 1 - \eta(k) & \text{if } k = i \\ \eta(k) & \text{if } k \neq i \end{cases} \qquad (3.6)$$

To be definite we take births and deaths only at the boundary sites $i = -N, N$.

The physical interpretation of the dynamics is quite simple. Think of a one-dimensional channel in which particles diffuse while they enter or leave the system at its boundary. A biophysical realization seems to be found in the physics of ion channels connecting the inside and the outside of a living cell. The channel is a sort of opening or gate in the cell's membrane through which charged particles can move from higher to lower concentration, or following the gradient in electric potential etc. Here the relevant parameters are the values $a_{\pm N}$ which in fact represent the (different) chemical potentials of the two reservoirs at the outer edges.

With these definitions the Master equation governing the temporal behavior of probability measures on K is given by

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{P}_t(\eta) = &\sum_{i=1}^{N-1}[C(i, i+1, \eta^{i,i+1})\mathbb{P}_t(\eta^{i,i+1}) - C(i, i+1, \eta)\mathbb{P}_t(\eta)] \\ &+ C(-N, \eta^{-N})\mathbb{P}_t(\eta^{-N}) - C(-N, \eta)\mathbb{P}_t(\eta) \\ &+ C(N, \eta^N)\mathbb{P}_t(\eta^N) - C(N, \eta)\mathbb{P}_t(\eta) \end{aligned} \qquad (3.7)$$

That equation shows how the probability to find a given configuration in the system evolves in time. Alternatively, the generator L is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle f(\eta_t)\rangle = \langle Lf(\eta_t)\rangle \qquad (3.8)$$

for functions ("observables") f on K, and where $\langle \cdot \rangle$ takes the expectation over the Markov process, including some (as yet unspecified)

initial distribution. Explicitly,

$$Lf(\eta) = \sum_{i=1}^{N} C(i, i+1, \eta)[f(\eta^{i,i+1}) - f(\eta)]$$
$$+ C(-N, \eta)[f(\eta^{-N}) - f(\eta)] + C(N, \eta)[f(\eta^N) - f(\eta)] \quad (3.9)$$

Let us make a simple exercise by plugging in $f(\eta) = \eta(i)$ for some fixed i and by taking $\beta = 0$ in (3.4)–(3.5). The corresponding evolution equation is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \eta_t(i) \rangle = \langle \eta_t(i-1) + \eta_t(i+1) - 2\eta_t(i) \rangle$$

when $i \neq -N, N$, while for $i = \pm N$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \eta_t(i) \rangle = \langle \eta_t(i \mp 1) - \eta_t(i) + e^{-a_i \eta_t(i)}[1 - 2\eta_t(i)] \rangle$$

Apparently, these equations are closed in the density variables $\langle \eta_t(i) \rangle$, $i \in \Lambda_N$. In particular, putting their left-hand sides equal to zero, we get the stationary value $\langle \eta(i) \rangle = Ci + D$ for some constants C and D that depend on N and on the values $a_{\pm N}$. One checks that $a_{-N} = a_N = a$ if and only if $C = 0$, $D = 1/(1 + \exp(-a))$. When $C \neq 0$, then there is a linear density profile with slope $\sim 1/N$. Obviously, when repeating that calculation for $\beta \neq 0$, we run into a difficulty: the equation for the $\langle \eta_t(i) \rangle$ is no longer closed but there is a coupling with higher order correlation functions such as $\langle \eta_t(i)\, \eta_t(i+1) \rangle$. That feature is very generally true and it implies that we cannot simply solve the equations.[8] The stationary distribution is in general only implicitly known, as solution of the (time-independent) Master equation (3.7) with the left-hand side set zero.

3.4. **Path-space measure.** One has to remember that a Markov process is a special probability distribution on paths. In our case, we have piecewise-constant paths. A path ω over the time-interval $[0, \tau]$ starts from an initial configuration η_0 after which it changes into $\eta_{t_1}, \eta_{t_2}, \ldots$ at random times $t_1, t_2, \ldots$ To be more precise we must add what is the configuration at the jump times as well. That is just a convention, and we take it that $\eta_{t_{k-1}} = \eta_{t_k-}$ and $\eta_{t_k} = \eta_{t_k+}$, or, the step-function is continuous from the right.

An important transformation on path-space concerns the so called time-reversal Θ in which $(\Theta\omega)_t = \omega_{\tau-t}$, up to irrelevant modifications at the jump times making $\Theta\omega$ again right-continuous.

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[8]The problem appears in all nontrivial dynamics for many particle systems. The resulting hierarchy of equations is sometimes referred to as the BBGKY-hierarchy, referring in particular to the hierarchy of equations that appear in kinetic gas theory for the various particle distribution functions. The study of possible ways of closing the hierarchy is a major concern in nonequilibrium physics.

The random times are called the jump times of the process. The Markov process assigns a probability law to these times and to the corresponding transitions. There are two ingredients: the waiting time and the transition step. The waiting time is exponentially distributed with a weight $\lambda(\eta)$ that depends on the present configuration η. That waiting time is directly (and inversely) related to the escape rate

$$\lambda(\eta) = \sum_{\eta'} W(\eta \to \eta')$$

We will use the notation $W(\eta \to \eta')$ when indicating one allowed but general transition rate.

The second ingredient sits in the transition rates as we have them introduced before. When the waiting time is over, a new configuration is chosen so that for time $t \downarrow 0$,

$$\text{Prob}[\eta_t = \eta' \mid \eta_0 = \eta] = (1 - \lambda(\eta)\, t)\, \delta_{\eta,\eta'} + W(\eta \to \eta')\, t + o(t)$$

A more explicit realization of that path-space measure goes via Girsanov's formula, see Section 6.

4. Steady state

4.1. **Detailed balance.** One observes from the definition (3.4) that:

$$\frac{C(i,j,\eta)}{C(i,j,\eta^{i,j})} = \frac{\exp\left[-\beta H\left(\eta^{i,j}\right)\right]}{\exp\left[-\beta H\left(\eta\right)\right]} = \frac{\mathbb{P}^{\beta,a}[\eta^{i,j}]}{\mathbb{P}^{\beta,a}[\eta]} \qquad (4.1)$$

where we have inserted the ratio of probabilities according to (3.2). That is verified for all values a. Furthermore, with the definition (3.5) we have

$$\frac{C(i,\eta)}{C(i,\eta^i)} = \frac{\exp[-a_i \eta(i)]}{\exp[-a_i(1 - \eta(i))]} \frac{\exp\left[-\beta H\left(\eta^i\right)\right]}{\exp\left[-\beta H\left(\eta\right)\right]}, \quad i = \pm N \qquad (4.2)$$

If $a_{-N} = a_N = a$ then

$$\frac{\exp[-a_i \eta(i)]}{\exp[-a_i(1 - \eta(i))]} = \frac{e^{a(1-\eta(i))}}{e^{a\eta(i)}}$$

Comparing with formula (3.2), still for $i = \pm N$ and for $a_{-N} = a_N = a$,

$$\frac{C(i,\eta)}{C(i,\eta^i)} = \frac{\mathbb{P}^{\beta,a}[\eta^i]}{\mathbb{P}^{\beta,a}[\eta]} \qquad (4.3)$$

Summarizing, when the particle reservoirs left and right have equal concentration, then the system dynamics satisfies the condition of detailed balance

$$\frac{W(\eta \to \eta')}{W(\eta' \to \eta)} = \frac{\mathbb{P}^{\beta,a}[\eta']}{\mathbb{P}^{\beta,a}[\eta]} \qquad (4.4)$$

for all allowed transitions $\eta \to \eta'$ and corresponding transition rates $W(\eta \to \eta')$. Under that same condition $a_{-N} = a_N = a$ we thus have

that (3.2) is a reversible stationary measure. The corresponding process is the steady state for equilibrium conditions.

Observe that if we consider unequal rates at the boundaries $a_1 \neq a_N$ then we could still try

$$\mathbb{P}^{\beta,a_1,a_N}(\eta) = \frac{1}{Z} \exp[-\beta H(\eta)] \exp[a_1 \eta(1) + a_N \eta(N)] \qquad (4.5)$$

as a candidate stationary distribution. In that case the analogue of (4.3) is still verified. Yet, the condition (4.1) fails.

4.2. **Nonequilibrium model.** Now comes the question what happens when $a_1 \neq a_N$. Let us first consider the left boundary of the system, for which we can write, see (4.2),

$$\frac{C(-N,\eta)}{C(-N,\eta^{-N})} = e^{-\beta[H(\eta^{-N})-H(\eta)]-a_{-N} J_\ell(\eta,\eta^{-N})} \qquad (4.6)$$

where $J_\ell(\eta,\eta^{-N}) = 1$ when the particle leaves the system via the site $-N$, i.e., $\eta(-N) = 1$, and $J_\ell(\eta,\eta^{-N}) = -1$ when a new particle enters, i.e., $\eta(-N) = 0$. That is an antisymmetric current of particles, taking positive when the particles leave the system. In the same way we define the current $J_r(\eta,\eta') = 1$ when $\eta(N) = 1$, $\eta' = \eta^N$ and $J_\ell(\eta,\eta') = -1$ when $\eta(N) = 0$, $\eta' = \eta^N$. The currents are zero otherwise.

Taking all transitions together, we have

$$\frac{W(\eta \to \eta')}{W(\eta' \to \eta))} = e^{-\beta[H(\eta')-H(\eta)]-a_{-N} J_\ell(\eta,\eta')-a_N J_r(\eta,\eta')} \qquad (4.7)$$

One recognizes the change of entropy in the environment:

$$S(\eta,\eta') = \beta \Delta E(\eta,\eta') - \mu_\ell \Delta \mathcal{N}_\ell(\eta,\eta') - \mu_r \Delta \mathcal{N}_r(\eta,\eta')$$

where $\mu_\ell = a_{-N}$ respectively $\mu_r = a_N$ are the chemical potentials (up to some factor β that we have ignored) of the particle reservoirs left and right, and $J_\ell = \Delta \mathcal{N}_\ell$, $J_r = \Delta \mathcal{N}_r$ are the changes in particle number in the *left*, respectively *right* particle reservoir. The form (4.7) or

$$\frac{W(\eta \to \eta')}{W(\eta' \to \eta)} = e^{S(\eta,\eta')}$$

is known as that of local detailed balance.[9]

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[9]Remark that in (4.7) a possible time-symmetric prefactor to the rates (3.5) or (3.4) will never appear; there is only the part that is antisymmetric under $\eta \leftrightarrow \eta'$. The fact that the entropy production appears as the source term of the breaking of time-reversal symmetry, is no accident but it is related to more general considerations that here are simply applied in order to obtain a reasonable physical interpretation of our effective dynamics, see e.g. [38, 40].

The currents J_ℓ and J_r appear in the conservation law for the particle number. The sum of these currents equals the number of particles that leave the system,

$$J_\ell(\eta, \eta') + J_r(\eta, \eta') = \mathcal{N}(\eta) - \mathcal{N}(\eta') \tag{4.8}$$

or

$$a_{-N} J_\ell(\eta, \eta') + a_N J_r(\eta, \eta') = (a_{-N} - a_N) J_\ell + a_N(\mathcal{N}(\eta) - \mathcal{N}(\eta')) \tag{4.9}$$

¿ From now on, we write $a_N = a$, $a_{-N} = a + \delta$ so that

$$\frac{W(\eta \to \eta')}{W(\eta' \to \eta)} = \frac{\mathbb{P}^{\beta,a}[\eta']}{\mathbb{P}^{\beta,a}[\eta]} e^{-\delta J_\ell(\eta, \eta')}$$

The parameter δ thus measures some distance to the equilibrium situation, and enables the tentative terminology of *close* versus *far* from equilibrium.

As above we define the bulk currents $J_i(\eta, \eta')$ to be $+1$ if in the transition $\eta \to \eta'$ a particle moves over the bond $i \to i + 1$, and equal to -1 if a particle moves $i \leftarrow i + 1$. More generally,[10] we consider a path $\omega = (\eta_t)_{t=0}^\tau$ and currents $J_i(\omega)$, $i = -N, \ldots, N$, defined by

$$J_i(\omega) = J_i(\eta_0, \eta_{t_1}) + J_i(\eta_{t_1}, \eta_{t_2}) + \ldots + J_i(\eta_{t_{n-1}}, \eta_\tau)$$

In particular, $J_r = J_N$ and for $i \leq k$,

$$J_i(\omega) - J_k(\omega) = \mathcal{N}_{[i+1,k]}(\eta_\tau) - \mathcal{N}_{[i+1,k]}(\eta_0)$$
$$J_\ell(\omega) + J_{-N}(\omega) = \eta_0(-N) - \eta_\tau(-N) \tag{4.10}$$

Observe that the currents J_i are extensive in the time τ.

All of that is related to the process, be it transient or be it steady. Except for the following section however, we will be mostly interested in the steady state regime. It is easy to verify that we have here a unique stationary distribution ρ. It satisfies the time-independent Master equation (3.7) (zero left-hand side). Corresponding to ρ there is then a stationary process with distribution $\boldsymbol{P}_\rho$. If we look at expectations in the stationary process we write $\langle \cdot \rangle_\rho$.
¿ From the conservation laws (4.8) and (4.10) we have

$$\langle J_\ell \rangle_\rho = -\langle J_r \rangle_\rho = -\langle J_i \rangle_\rho, \qquad i \in \Lambda_N$$

There are alternative expressions for these expectations by using the dynamical equations (3.8). For example, for $i \neq N, -N$,

$$\frac{1}{\tau}\langle J_i \rangle_\rho = \langle C(i, i+1, \eta)(\eta(i) - \eta(i+1)) \rangle_\rho = \langle 1 - \eta(N)[1 + e^{-a}] \rangle_\rho$$

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[10]In fact and throughout we call current what is more like a time-integrated current, or a change of particle number.

5. Time-dependent dynamics

5.1. **Modifications with respect to Section 4.** Nonequilibrium conditions can be obtained in a variety of ways. The above gives a set-up for boundary driven steady states. Another way of driving the system away from equilibrium is by applying an external *bulk* field. We consider here a modification which also frustrates the system (as it cannot simply relax to equilibrium). We remain with the same states but the updating becomes time-dependent. The idea is that the values of parameters in the Hamiltonian are changed while the dynamics enrolls.

We have a time-dependent Hamiltonian H_t so that the transition rates $W_t(\eta \to \eta')$ are also depending on the moment t of the jump $\eta \to \eta'$. For example, the rate for exchanging the occupation at sites i and $j = i \pm 1$ is

$$C_t(i, j, \eta) = \exp\left[-\frac{\beta}{2}\left(H_t(\eta^{i,j}) - H_t(\eta)\right)\right], \qquad |i - j| = 1 \qquad (5.1)$$

(compare with (3.4)) depending on the time t.
There is no longer a very good sense in which we can speak about the stationary distribution. Still we can consider for each H_t, $t \in [0, \tau]$, the corresponding Gibbs distribution

$$\rho_t(\eta) = \frac{1}{\mathcal{Z}_t} \, e^{a \sum \eta(i)} \, e^{-\beta H_t(\eta)} \qquad (5.2)$$

where $\mathcal{Z}_t = \mathcal{Z}_t(a, \beta, N)$ is now also time-dependent. There is an associated free energy

$$\mathcal{A}_t = -\frac{1}{\beta} \log \mathcal{Z}_t \qquad (5.3)$$

In the time-dependent case, we will only work with the dynamics for which $\delta = 0$, $a_{-N} = a_N = a$ fixed, i.e., there is just one particle reservoir and one heat bath reservoir.[11]

5.2. **Work and heat.** When there is an energy exchange between system and reservoir, there is heat. For a history $\omega = (\eta_t)_0^\tau$ where the jumps in the configuration happen at times $t_1, t_2, \ldots t_n$, the total heat $\mathcal{Q}$ transferred to the system is the sum of differences of energy:

$$\mathcal{Q} = H_{t_1}(\eta_{t_1}) - H_{t_1}(\eta_0) + H_{t_2}(\eta_{t_2}) - H_{t_2}(\eta_{t_1}) + \ldots$$
$$+ H_{t_n}(\eta_\tau) - H_{t_n}(\eta_{t_{n-1}}) \qquad (5.4)$$

---

[11]We can of course make a dynamics such that at every moment the distribution $\mathbb{P}_t = \rho_t$ exactly coincides with (5.2). We could e.g. take a transition rate $\bar{W}_t(\eta \to \eta') = \rho_t(\eta')$. One can think of it as admitting an infinitely fast relaxation of the equilibrium process. Alternatively, one can think of an ultra-slow time-dependence in H_t so that, before any change, the system has already relaxed to the equilibrium distribution corresponding to the instantaneous value.

On the other hand, the work $\mathcal{W}$ performed upon the system is a sum of changes of the Hamiltonian at fixed configurations:

$$\mathcal{W} = H_\tau(\eta_\tau) - H_{t_n}(\eta_\tau) + H_{t_n}(\eta_{t_{n-1}}) - H_{t_{n-1}}(\eta_{t_{n-1}}) + \dots$$
$$+ H_{t_1}(\eta_0) - H_0(\eta_0) \qquad (5.5)$$

Therefore, as an expression of the first law of thermodynamics,

$$\mathcal{Q} + \mathcal{W} = H_\tau(\eta_\tau) - H_0(\eta_0) \qquad (5.6)$$

is the total change of system energy between the initial and the final configurations η_0 and η_τ in the path ω.

6. Lagrangian set-up: Girsanov formula

As we have seen in the course of our computation around and below (3.9), the evolution equations give a hierarchy of equations for the various correlation functions of the stationary distribution. Solving them is like diagonalizing a large matrix and it is not even clear whether it would always permit us to extract the most relevant information. A more global characterization of the stationary distribution is perhaps obtained by going to a space-time picture. On that level the process is space-time local and explicit. The variables are the histories or trajectories of the system.

Given two Markov processes on the same space K, we can consider two path-space measures $\boldsymbol{P}$ and $\bar{\boldsymbol{P}}$ with corresponding escape rates λ and $\bar{\lambda}$, and transition rates W and $\bar{W}$. We consider all paths on the interval $[0, \tau]$ and we assume that for all η,

$$\{\eta', W(\eta \to \eta') \neq 0\} = \{\eta', \bar{W}(\eta \to \eta') \neq 0\}$$

We can then look for the density of $\boldsymbol{P}$ with respect to $\bar{\boldsymbol{P}}$. That density is a Radon-Nikodym derivative and can be written down quite explicitly in the so called Girsanov formula:

$$\frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}\bar{\boldsymbol{P}}}(\omega) = \exp\left[\int_0^\tau \left(\lambda(\eta_t) - \bar{\lambda}(\eta_t)\right) \mathrm{d}t + \sum_{t \leq \tau} \log \frac{W(\eta_{t-} \to \eta_t)}{\bar{W}(\eta_{t-} \to \eta_t)}\right] \quad (6.1)$$

when restricted to events that are measurable from the trajectory in $[0, \tau]$. The last sum in the exponential is over the jump times, as they appear in the path ω. We have assumed here that the two processes $\boldsymbol{P}$ and $\bar{\boldsymbol{P}}$ start from the same configuration. If they have different initial distributions ν and $\bar{\nu}$, then a prefactor $\nu(\eta)/\bar{\nu}(\eta)$, $\omega_0 = \eta$, must be added to the right-hand side of the Girsanov formula (6.1). The formula remains intact when the process is not time-homogeneous. One

then adds the correct time-dependence to the escape and to the transition rates.[12]

Our application of the Girsanov formula will concern time-reversal. If we have a distribution $\boldsymbol{P}$ on paths, then its time-reversal $\boldsymbol{P}\Theta$ is obtained via

$$\frac{\mathrm{d}\boldsymbol{P}\Theta}{\mathrm{d}\boldsymbol{P}^0}(\omega) = \frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}\boldsymbol{P}^0}(\Theta\omega)$$

for an arbitrary process $\boldsymbol{P}^0$ which is reversible. The dependence on initial configurations is again ignored, but it is essential in the consideration of the time-reversal invariant process $\boldsymbol{P}^0$.

7. FLUCTUATION RELATIONS FOR THE ENTROPY PRODUCTION

7.1. **Jarzynski equality.** Recall the set-up for the time-dependent dynamics in Section 5. We take the case where $a_1 = a_N = a$. The Jarzynksi identity is a relation between the work $\mathcal{W}$ of (5.5) and the change in free energy (5.3). In the context of stochastic lattice gases, we get it as

$$\mathbb{E}^a_{\rho_0}[e^{-\beta\mathcal{W}}] = e^{-\beta\Delta\mathcal{A}}, \tag{7.1}$$

The left-hand side is the expectation in the time-dependent dynamics with fixed chemical potential (left and right) equal to a and with Hamiltonian H_t at inverse temperature β, started from equilibrium ρ_0 at time $t = 0$. The right-hand side contains the difference

$$\Delta\mathcal{A} = \mathcal{A}_\tau - \mathcal{A}_0, \tag{7.2}$$

of free energies[13] (5.3).

Proof. To prove (7.1) we make a first application of the Girsanov formula. The two distributions correspond to our time-dependent process $\boldsymbol{P}^a_{\rho_0}$ on the one hand and to the time-reversed process $\bar{\boldsymbol{P}}^a_{\rho_\tau}\Theta$ on the

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[12]The formula is also not really restricted to Markov processes, or to finite state spaces. The more useful way of considering that formula is as a generalization of the Boltzmann-Gibbs formula (3.2), where the essential input is that one can make sense of what is written in the exponential as a sum of quasi-local terms. Here we can speak about the action as a sum of a local Lagrangian. Indeed, if we write out the rates $W(\eta \to \eta')$ of our stochastic lattice gas, and we take $\bar{\boldsymbol{P}}$ say corresponding to $\beta = 0$, $a_{-N} = a_N = 0$ we obtain there a sum over space-time of local interaction terms. Without trying to formalize the idea, see however [39], one can thus consider the stationary distribution to be the projection (or restriction) of that space-time path-space measure to an equal time layer, see e.g. [34]. There is no *a priori* reason why that projected measure should inherit a spatial locality, see e.g. [44].

[13]To make sure, there is no assumption that at any future time $t > 0$ (including at time τ) the distribution should be the ρ_t of (5.2). We are starting from equilibrium at time zero, but then the system is most likely away from instantaneous equilibrium with respect to the Hamiltonian H_t. Yet, the result of (7.1) is a statement about equilibrium free energies. We can measure these (and how they possibly depend on some parameter) via some nonequilibrium procedure.

other hand. By $\bar{\boldsymbol{P}}^a_{\rho_\tau}$ we mean the process started at time zero from the distribution ρ_τ and with time-reversed protocol, i.e., the rates are $\bar{W}_t = W_{\tau-t}$.

We have therefore for a fixed path ω with jump times $t_1, \ldots, t_n$ in the interval $[0, \tau]$, that

$$\frac{\mathrm{d}\boldsymbol{P}^a_{\rho_0}}{\mathrm{d}\bar{\boldsymbol{P}}^a_{\rho_\tau}\Theta}(\omega) = \frac{\rho_0(\omega_0)}{\rho_\tau(\omega_\tau)} \, \exp R(\omega) \tag{7.3}$$

with, from (6.1),

$$R = \frac{W_{t_1}(\eta_0 \to \eta_{t_1})W_{t_2}(\eta_{t_1} \to \eta_{t_2}) \ldots W_{t_n}(\eta_{t_{n-1}} \to \eta_\tau)}{W_{t_n}(\eta_\tau \to \eta_{t_{n-1}}) \ldots W_{t_2}(\eta_{t_2} \to \eta_{t_1})W_{t_1}(\eta_{t_1} \to \eta_0)} \tag{7.4}$$

By using the detailed balance relations

$$\frac{W_t(\eta \to \eta')}{W_t(\eta' \to \eta)} = \exp[-\beta(H_t(\eta') - H_t(\eta)) + a(\mathcal{N}(\eta') - \mathcal{N}(\eta))]$$

and combining that with the expression (5.4) for the heat, the ratio (7.4) reduces to

$$R(\omega) = e^{-\beta\mathcal{Q}} \, e^{a[\mathcal{N}(\eta_\tau) - \mathcal{N}(\eta_0)]}$$

Hence, looking back at (7.3) and substituting (5.2), (5.6) and (7.2), we have

$$\log \frac{\mathrm{d}\boldsymbol{P}^a_{\rho_0}}{\mathrm{d}\bar{\boldsymbol{P}}^a_{\rho_\tau}\Theta}(\omega) = -\beta\mathcal{Q}(\omega) + \log \frac{\mathcal{Z}_\tau}{\mathcal{Z}_0} - \beta[H_0(\eta_0) - H_\tau(\eta_\tau)]$$

$$= \beta[\mathcal{W}(\omega) - \Delta\mathcal{A}] \tag{7.5}$$

The Jarzynski equality (7.1) is then an easy consequence of the normalization of path-space measures:

$$\int \mathrm{d}\boldsymbol{P}^a_{\rho_0}(\omega)\frac{\mathrm{d}\bar{\boldsymbol{P}}^a_{\rho_\tau}\Theta}{\mathrm{d}\boldsymbol{P}^a_{\rho_0}}(\omega) = 1 \tag{7.6}$$

$\square$

For further background information on these relations between irreversible work and free energy differences, one can check e.g. [7, 25, 38].

7.2. **The direction of particle current.** We come back to the time-homogeneous nonequilibrium process as we had it first in Section 4.2. Physically we expect that there will be a particle current flowing from higher to lower concentration. To be specific, let us assume that $\delta \geq 0$, $a_{-N} \geq a_N$, so that the physical picture suggests that the mean particle current $\langle J_i \rangle_\rho \geq 0$. The question is how to actually see that. Remember that we do not know a thing about the stationary distribution ρ in general. Nevertheless the direction of the particle current will easily follow within our set-up.

¿ From the Girsanov formula (6.1) for $\boldsymbol{P}_\rho$ with respect to $\boldsymbol{P}_\rho\Theta$, both started in the stationary distribution ρ, we have

$$\frac{\mathrm{d}\boldsymbol{P}_\rho}{\mathrm{d}\boldsymbol{P}_\rho\Theta}(\omega) = \frac{\rho(\omega_0)}{\rho(\omega_\tau)} \exp\left[-\beta\left(H(\omega_\tau) - H(\omega_0)\right) + a\Delta\mathcal{N} - \delta J_\ell(\omega)\right],$$

(7.7)

Again from the normalization we have:

$$\int \mathrm{d}\boldsymbol{P}_\rho(\omega)\frac{\mathrm{d}\boldsymbol{P}_\rho\Theta}{\mathrm{d}\boldsymbol{P}_\rho}(\omega) = 1.$$

and hence, by concavity,

$$\int \mathrm{d}\boldsymbol{P}_\rho(\omega)\log\frac{\mathrm{d}\boldsymbol{P}_\rho\Theta}{\mathrm{d}\boldsymbol{P}_\rho}(\omega) \le 0.$$

But, from (7.7) and by stationarity

$$0 \le \int \mathrm{d}\boldsymbol{P}_\rho \log\frac{\mathrm{d}\boldsymbol{P}_\rho}{\mathrm{d}\boldsymbol{P}_\rho\Theta}(\omega) = -\delta\langle J_\ell\rangle_\rho = \delta\langle J_i\rangle_\rho$$

(7.8)

We conclude that

$$\delta\langle J_i\rangle_\rho \ge 0$$

(7.9)

which shows that the average direction of the particle current depends only on the sign of δ. See [42] for a very similar analysis in the case of heat conduction.

To get a strict inequality $\langle J_i\rangle_\rho > 0$ is also possible for $\delta > 0$; it suffices to see that there is a non-zero probability that the current J_i as a function of the path ω is not constant equal to zero even when $\omega_0 = \omega_\tau$.

7.3. **Fluctuation theorem.** The previous results were all a direct consequence of the normalization condition applied to the Radon-Nikodym derivative (6.1) between two path-space measures. Here we go for a result that is somewhat more detailed and concerns a symmetry in the fluctuations of the current. We follow the method of [38, 39, 43] but the present model can also be treated via [35].

We fix an $i = -N, \ldots, N$ and consider the current J_i as function of the path over the interval $[0, \tau]$. Define the generating function $q(\lambda)$, $\lambda \in \mathbb{R}$ by

$$q(\lambda) = \lim_{\tau\uparrow+\infty} \frac{1}{\tau}\log\langle e^{-\lambda J_i}\rangle_\rho$$

(7.10)

The limit exists by the Perron-Frobenius theorem, and is independent of $i = -N, \ldots, N$ because of (4.10). The fluctuation symmetry is that

$$q(\lambda) = q(\delta - \lambda)$$

(7.11)

Before providing a proof observe that $q(\lambda)$ is the Legendre transform of the rate functions of large deviations for J_i. The interested reader

is referred to the literature on large deviations (and the Gärtner-Ellis theorem in particular) for more details, see e.g. [9]. The idea is that

$$\boldsymbol{P}_\rho[J_i \simeq \tau j] \simeq e^{-\tau I(j)}, \qquad \tau \to +\infty \tag{7.12}$$

with

$$I(j) = \inf_\lambda(-\lambda j - q(\lambda)) \tag{7.13}$$

Substituting the identity (7.11), we get

$$I(j) = \inf_\lambda \left((-\delta + \lambda)(-j) - q(\delta - \lambda)\right) - \delta\, j = -\delta\, j + I(-j) \tag{7.14}$$

or

$$I(j) - I(-j) = -\delta\, j \tag{7.15}$$

That can be again translated to an identity for (7.12):

$$\frac{\boldsymbol{P}_\rho(J_i/\tau \simeq j)}{\boldsymbol{P}_\rho(J_i/\tau \simeq -j)} \simeq e^{\tau\,\delta\,j} \tag{7.16}$$

The interpretation of that expression is that there exists a relation between the probabilities of having a current $+j$ and $-j$; the probability of having a particle current in the direction opposite to the expected one ($\delta j > 0$) is exponentially small with $\tau \to +\infty$. The formula (7.16) has appeared before and many papers have been devoted to proving it in a variety of contexts. It first appeared in the context of smooth dynamical systems where it concerned the fluctuations of the phase space contraction, [17, 16, 50], and the result has become known as the (steady state) fluctuation theorem.

We now prove (7.11).

Proof. By definition and since $J_i(\Theta\omega) = -J_i(\omega)$,

$$\langle e^{-\lambda J_i}\rangle_\rho = \int \mathrm{d}\boldsymbol{P}_\rho(\Theta\omega)\, e^{\lambda J_i(\omega)}$$

Next we insert the Radon-Nikodym derivative

$$\int \mathrm{d}\boldsymbol{P}_\rho(\omega)\frac{\mathrm{d}\boldsymbol{P}_\rho\Theta}{\mathrm{d}\boldsymbol{P}_\rho}(\omega)\, e^{\lambda J_i(\omega)} = \int \mathrm{d}\boldsymbol{P}_\rho(\omega)\exp[\Delta + \delta J_i(\omega)]\, e^{\lambda J_i(\omega)} \tag{7.17}$$

where, via (6.1) or via (7.7),

$$\Delta = \log\frac{\rho(\omega_\tau)}{\rho(\omega_0)} + \beta\left(H(\omega_\tau) - H(\omega_0)\right) - a\Delta\mathcal{N} + \delta(J_\ell(\omega) + J_i(\omega)) \tag{7.18}$$

Notice that $|\Delta\mathcal{N}| = |\mathcal{N}(\omega_\tau) - \mathcal{N}(\omega 0)| \le 2N$. Further, $|\log \rho(\omega_\tau)/\rho(\omega_0)|$ is also bounded because at any rate, $\rho(\eta) \ne 0$, $\eta \in K$. Finally, there is the conservation law

$$J_\ell(\omega) + J_i(\omega) = -N_{[-N,i]}(\omega_\tau) + N_{[-N,i]}(\omega_0) \tag{7.19}$$

implying that the sum of these currents is also bounded, and $|H(\omega_\tau) - H(\omega_0)| \le 4(\kappa + B)N$, see (3.1). Hence we conclude that $|\Delta| \le \text{const}$ (with a constant that also depends on N but not on τ) which finishes the proof. $\qquad\square$

In the case $\beta = 0$ (the bulk dynamics is that of the so called simple symmetric exclusion process), more is known about the fluctuations of the current, see e.g. [13].

8. More nonequilibrium issues

Only a limited review has been given in the previous sections of recent work on nonequilibrium aspects of stochastic lattice gases. We attempt to give some additional remarks.

8.1. **Escape from equilibrium.**
Imagine yourself enclosed in a well-isolated room. At time zero somebody opens doors and windows; how long would it take before you feel that? Probably you will become aware of the openings because of some air current, and its intensity will depend on the outdoor conditions.

In the present section we use our model to ask a similar question. Suppose a probability distribution μ on K which is nonzero, $\mu(\eta) > 0$, only when $\mathcal{N}(\eta) = m$ for some given number $0 < m < N$ of particles. For the rest we assume that it is thermally distributed:[14]

$$\mu(\eta) = \frac{1}{\mathcal{Z}_m} \exp[-\beta H(\eta)] \, \chi(\mathcal{N}(\eta) = m) \tag{8.1}$$

We consider the dynamics of Section 4.2 in the steady state $\boldsymbol{P}_\rho$ and we ask for the fraction of times that we see a fixed configuration η:

$$p_\tau(\eta) = \frac{1}{\tau} \int_0^\tau \chi(\eta_t = \eta) \, \mathrm{d}t$$

That time-average is a random variable (depends on η). An important question in the theory of large deviations is to ask whether these fractions resemble a given probability measure; here we ask what is the function $I(\mu)$ so that

$$\boldsymbol{P}_\rho[p_\tau \simeq \mu] \simeq e^{-\tau \, I(\mu)}, \qquad \tau \uparrow +\infty \tag{8.2}$$

That question has been rigorously studied by Donsker and Varadhan, [9, 14], and we know an expression for $I(\mu)$:

$$I(\mu) = -\inf_{g>0} \left\langle \frac{Lg}{g} \right\rangle_\mu \tag{8.3}$$

The expectation is over the distribution μ and Lg is as before the generator of the process acting on a function g (over which we vary in (8.3)). It is known that in the case of a detailed balance process, the minimizer in (8.3) is $g^\star = \sqrt{\mu/\rho}$.

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[14]χ is the indicator function.

¿ From (8.3) it is clear that we must find the function g on K that minimizes

$$\sum_{\eta \in K} \frac{\mu(\eta)}{g(\eta)} \Big[\sum_{i=1}^{N-1} C(i, i+1, \eta)\, g(\eta^{i,i+1}) + g(\eta^{-N})\, C(-N, \eta) + g(\eta^{N})\, C(N, \eta) \Big]$$

The sum is effectively over all η with $\mu(\eta) > 0$ or $\mathcal{N}(\eta) = m$. Since the configurations $\eta^{\pm N}$ have one particle more or less than η, we can put $g(\xi) = 0$ whenever $\mathcal{N}(\xi) \neq m$, and the minimization is over

$$\sum_{\eta \in K} \frac{\mu(\eta)}{g(\eta)} \sum_{i=1}^{N-1} C(i, i+1, \eta)\, g(\eta^{i,i+1})$$

Taking again the complete Donsker-Varadhan functional we have

$$I(\mu) = \langle C(-N, \eta(-N)) + C(N, \eta(N)) \rangle_{\mu} - \inf_{g} \Big\langle \frac{\mathcal{L}g}{g} \Big\rangle_{\mu} \qquad (8.4)$$

where the new generator $\mathcal{L}$ only considers particle exchanges generating a dynamics that satisfies the condition of detailed balance with respect to our μ; in other words, it is typical to 'see' the distribution μ for that pure hopping process. It follows that the second term in (8.4) is zero to conclude that

$$I(\mu) = \langle C(-N, \eta(-N)) + C(N, \eta(N)) \rangle_{\mu}$$

The issue here is somewhat related to the problem of metastability, as found also in the contributions by Anton Bovier and by Frank den Hollander, see also [4]. At the same time, it is related to e.g. Section 5.7 in [9] (diffusion from a domain), and from a physics point of view it is related to Kramers' theory, [22].

8.2. **Macroscopic fluctuations.** The previous calculation is related to the theory of dynamical fluctuations. There is however another scale of description on which similar questions become better manageable, that is the level of macroscopic fluctuations, static and dynamical. For our model, it refers to a hydrodynamical scaling in which one observes the evolution of the density profile. After a diffusive space-time rescaling one finds that the density profile $n_t(r)$ obeys a standard diffusion equation, [30],

$$\frac{\partial n_t(r)}{\partial t} = \frac{1}{2} \frac{\partial}{\partial r} D(n_t(r)) \frac{\partial}{\partial r} n_t(r), \qquad r \in [-1, 1]$$

where $D(n_t(r))$ is the diffusion 'constant,' further constrained by imposing the boundary conditions $\rho(\pm 1) = 1/(1 + e^{a \pm})$. In the simplest case (corresponding to $\beta = 0$) the diffusion is truly constant and the stationary profile $n^{\star}$ is linear. One can however ask for fluctuations around that (typical) behavior. The hydrodynamic equation is the result of a law of large numbers and we can ask for the plausibility of

a deviating density profile. We refer to [1, 13, 31, 41] for further results and insights.

Part II.
Macroscopic irreversibility

9. Introduction

Up to now we have been discussing so called mesoscopic systems, or more precisely, classical mesoscopic systems modeled as stochastic processes. Time-reversal symmetry was broken by applying external conditions, frustrating the system in its return to equilibrium. However, the microscopic laws of nature are time-reversal invariant. One could then perhaps have expected to find that all resulting behavior is invariant under time-reversal, except perhaps for some microscopic interactions.[15] That is not what we see: systems return to equilibrium thereby showing the infamous arrow of time. The equations of macroscopic physics are not time-reversible (or not always). They have often been described and been used quite some time before their microscopic origin was clarified. In fact their (macroscopic) irreversibility once casted doubt on the kinetic and atomistic picture of matter and motion. One of the greatest successes in the pioneering days of statistical mechanics was then indeed the explanation of that manifest irreversibility.

That the emergent macroscopic laws are irreversible is not so difficult to understand at least qualitatively. One should realize that distinct macroscopic states can be very different in the number of microstates they consist of. It is the installation of an initial macrostate that breaks the invariance under time-reversal: unless forbidden by additional constraints, a less plausible initial state evolves to a more plausible macrostate and finally to the most plausible, called equilibrium, exactly because that is more plausible. The plausibility is measured in terms of the 'number' of microstates or, more precisely, by the Boltzmann or counting entropy which has a well defined thermodynamic limit (a precise meaning of that counting needs to be and will be specified). The generic increase of the entropy between initial and final macrostates (traditionally both in equilibrium) is known as the second law of thermodynamics and can be formulated in various ways. Still, even more is often true: considerations of entropy via counting the microstates consistent with a given macrostate, are *a priori* not restricted only to the initial and the final states and can be applied to each intermediate, 'nonequilibrium' state as well. Extended in that way, the Boltzmann entropy is often an increasing function of time, as was first demonstrated for the Boltzmann equation, the macroscopic

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[15]All would probably agree e.g. that the weak fundamental interaction is not at all responsible for macroscopic irreversibility, and most would probably agree that quantum mechanics is not either (while this is somewhat more tricky).

evolution equation for rare gases, and rigorously proven in the so called Boltzmann-Grad scaling limit and for short times by Lanford, [32]. Such a much more detailed or 'microscopic' version of the second law proves to be valid much beyond the Boltzmann equation; for general theoretical arguments see [26, 27, 28, 18, 20, 21, 48].

¿ From a mathematical point of view, the second law in the form of an H-theorem in fact claims the existence of a Lyapunov functional for a class of evolution equations, and it even hints at how to find that: if we know the underlying microscopic dynamics from which the evolution equation (presumably or provably) follows, one is to search for the Boltzmann entropy. Understanding why this strategy often works brings to the foreground some other important observations: the validity of a macroscopic evolution equation means that there is a *typical* macroscopic behavior in the sense that it is a result of some law of large numbers. The fact that the macroscopic equation is often first order in time means that this macroscopic behavior is *autonomous*. On the other hand, the existence of microscopic configurations violating that typical macroscopic law is not only allowed but in a sense it is even *necessary* for a true irreversible behavior and a strict increase of entropy to occur! When formulated somewhat more precisely, these observations answer various apparent paradoxes as formulated by Loschmidt and Zermelo; a qualitative discussion can be found on various places, see e.g. [33, 6, 26].

Putting these arguments on a mathematically more precise level is relatively simple but it remains very instructive. First, in Section 10, we study a model introduced by Mark Kac, [29]. The arguments are formulated in a substantially more generality in Section 11 (the case of infinite dynamical systems) and Section 12 (the case of large but finite systems). In particular, we explain how an H-theorem follows from the very existence of an autonomous macroscopic dynamics. The resolution of Zermelo's and Loschmidt's paradoxes is understood via a fluctuation symmetry, in this way drawing a link to the first part of these lectures. Most of the presented material and some more details can be found in [11] and references therein.

Since the fundamental laws of nature are presumably quantum, one can further ask how the classical arguments leading to H-theorems need to be changed when starting from a quantum microscopic dynamics. There is no crucial difference up to one important point, namely that the very notion of a macroscopic state needs to be reconsidered because it can be (and in nonequilibrium practice it often *is*) specified through values of mutually incompatible observables. The non-commutativity is a genuine quantum-mechanical feature which cannot be simply waived away by arguments identifying the classical limit

with the thermodynamic limit. Furthermore, entropic arguments and microscopic derivations all together play on the level of fluctuations, i.e. before the thermodynamic limit. Starting from Section 13, we explain a possible approach to the quantum problem along the lines of reference [12], thereby generalizing some ideas of John von Neumann, [46]. An interesting side problem is to show how our construction of the quantum Boltzmann entropy relates to other, mathematically simpler but physically *a priori* less plausible constructions. In fact, we show when two definitions of quantum entropies become equivalent in the large system limit. That issue is obviously very related to the problem of quantum large deviations and we will briefly describe the connections. Finally, as an example, we come back to the Kac ring model and we discuss its quantum extension along the lines of reference [10]; see Section 14.

10. Kac ring model

There is a simple paradigmatic model introduced by Mark Kac [29] to simplify the mathematics of the Boltzmann equation. While the Boltzmann equation is much more complicated, the Kac model is mathematically simple and free of those extra technical problems that are not really important for understanding some crucial aspects of the emergence of macroscopic irreversibility.

10.1. **Microscopic dynamics.** Consider the set $\Lambda = \{1, \ldots, N\}$. We imagine it as a ring in which we identify the sites $1 = N + 1$ and on each site we have one particle and one scatterer. The particles carry a 'spin' $\eta(i) = \pm 1$ and the scatterers can be off or on, $g(i) \in \{0, 1\}$. The resulting set $K = \{-1, 1\}^\Lambda \times \{0, 1\}^\Lambda$ is the state space of our model. The dynamics is deterministic and given via the transformation U on K,

$$(U(\eta, g))(i) = ([1 - 2g(i - 1)] \, \eta(i - 1), \, g(i)) \mod N \qquad (10.1)$$

which generates the (microscopic) deterministic dynamics such that the configuration (η_t, g_t) at time $t = 0, 1, \ldots$ is

$$\eta_t(i) = \eta_0(i - t)[1 - 2g(i - t)] \ldots [1 - 2g(i - 1)] \qquad (10.2)$$

and $g_t = g$ keeps constant. There is an obvious interpretation: at every time instance t, each spin $\eta_t(i)$ jumps to its successive site, $i + 1$, either flipping its value if a scatterer is present, $g(i) = 1$, or keeping its value if $g(i) = 0$. Sampling the initial configuration (η_0, g) from a measure μ_0 on K, the probability to find (η, g) at time t is

$$\mu_t[(\eta, g)] = \mu_0[(\eta_t, g)] \qquad (10.3)$$

That is the present variant of the Liouville equation for mechanical systems. Here also the Shannon entropy $S(\mu) = -\sum_{\eta, g} \mu[(\eta, g)] \log \mu[(\eta, g)]$ is time-invariant, $S(\mu_t) = S(\mu_0)$. There is just no strictly increasing

Lyapunov function for this dynamical system; in fact, the dynamics is $2N-$periodic. Nevertheless the model exhibits relaxation to equilibrium; to see that, we need to pass to a macroscopic viewpoint.

10.2. **Macroscopic evolution.** There are two natural macroscopic observables, the magnetization m^N and the fraction of on-scatterers ρ^N:

$$m^N = \frac{1}{N} \sum_{i=1}^{N} \eta(i) \,, \qquad \rho^N = \frac{1}{N} \sum_{i=1}^{N} g(i) \qquad (10.4)$$

The emergent *macroscopic* dynamics will have the form

$$(m_t^N, \rho^N) \mapsto (m_{t+1}^N, \rho^N) = \phi(m_t^N, \rho^N) \qquad (10.5)$$

at least for very large N. It would imply that the macroscopic data (m_t^N, ρ_t^N) evolve *autonomously*, irrespectively of any actual microscopic configuration (η_t, g_t) that realize (10.4). A simple heuristics[16] suggests $\phi(m, \rho) = ([1 - 2\rho]m, \rho)$ as a candidate map. Yet, it is easy to imagine microscopic configurations that violate that and the question arises how such a macroscopic behavior can/must be understood.

Introducing the counting probability measures

$$\mathbb{P}^N[(\eta, g)] = 2^{-2N} \qquad (10.6)$$

and the notation $a \overset{\delta}{=} b$ for $|a - b| \leq \delta$, the desired statement has the form of a law of large numbers:[17]

$$\lim_{N\uparrow\infty} \mathbb{P}^N[m^N(\eta_t) \overset{\delta}{=} m_0(1 - 2\rho)^t \,|\, m^N(\eta_0) = m_0; \, \rho^N(g) = \rho] = 1 \quad (10.7)$$

for all $\delta > 0$. This means there is a set of *typical* microscopic configurations satisfying the macroscopic law with map ϕ; those configurations violating that law make a set of zero limit measure. Such a macroevolution is called *autonomous*; note that (10.7) is equivalent to

$$\lim_{N\uparrow\infty} \mathbb{P}^N[\forall t \leq T : m^N(\eta_t) \overset{\delta}{=} m_0(1-2\rho)^t \,|\, m^N(\eta_0) = m_0; \, \rho^N(g) = \rho] = 1$$
$$(10.8)$$

for all $\delta > 0$ and any finite T.

The relaxation to equilibrium along that typical macroevolution is obvious by inspection but one can also construct an explicit witness

---

[16] Think of $N(1 \pm m)$ up (down) spins crossing 'on average' $N\rho$ scatterers every time step, entirely neglecting possible time correlations. Such a hand-waving derivation is often referred to as *Stosszahlansatz* (or repeated randomization, molecular chaos approximation,...).

[17] In fact, a strong law of large numbers is also true for this model, see [29], but the weak law is sufficient for our purposes. Later we will meet an even substantially weaker autonomy condition.

which is the *Boltzmann entropy* $s(m, \rho)$ defined as the large deviation rate function for the sequence $(m^N, \rho^N)_{N\uparrow+\infty}$ of observables:

$$\mathbb{P}^N[(m^N(\eta), \rho^N(g))] \simeq (m, \rho)] \simeq e^{Ns(m,\rho)} \qquad (10.9)$$

This is to be understood in the logarithmic sense after taking the limit $N \uparrow +\infty$, i.e., it is a shorthand for the limit statement

$$s(m, \rho) = \lim_{\delta\downarrow0} \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathbb{P}^N[m^N(\eta) \overset{\delta}{=} m; \rho^N(\eta) \overset{\delta}{=} \rho] \qquad (10.10)$$

This is simply the binomial entropy,

$$s(m, \rho) = \begin{cases} -\frac{1+m}{2} \log(1 + m) - \frac{1-m}{2} \log(1 - m) \\ \qquad -\rho \log 2\rho - (1 - \rho) \log 2(1 - \rho) & \text{if } -1 < m < 1, \, 0 < \rho < 1 \\ -\infty & \text{otherwise} \end{cases} \qquad (10.11)$$

and one checks that $s(\phi(m, \rho)) > s(m, \rho)$ whenever $m \neq 0$ (system off equilibrium) and $0 < \rho < 1$ (nonsingular macrodynamics). Using the notation $m_t = m_0(1-2\rho)^t$, it yields that $s(m_t, \rho)$ is a strictly increasing function of time. Following Boltzmann's terminology, such a statement is called an *H-theorem*; the Boltzmann entropy is a Lyapunov function.

It should be clear that we say nothing yet about possible macroevolutions corresponding to those exceptional microstates not verifying the macroscopic map ϕ. That will come in Section 10.3.

Proof (10.7): Use the shorthand

$$\tilde{\mathbb{E}}^N[\,\cdot\,] = \mathbb{E}^N[\,\cdot\,|\, m^N(\eta_0) = m_0; \, \rho^N(g) = \rho]$$

for the expectations conditioned on the initial macrostate (m_0, ρ). One easily checks that (1) $\mathbb{P}^N$ are permutation-invariant measures, (2) η_0 and g are independently distributed under $\mathbb{P}^N$, and (3) the following asymptotic decoupling is true:[18] provided that $-1 < m_0 < 1$ and $0 < \rho < 1$, there is a sequence $\Delta_N^{(k)}$, $\lim_N \Delta_N^{(k)} = 0$ for all $k = 1, 2, \ldots$, such that

$$|\tilde{\mathbb{E}}^N[\eta(i_1) \ldots \eta(i_k)] - (\tilde{\mathbb{E}}^N[\eta(1)])^k| \leq \Delta_N^{(k)} \qquad (10.12)$$

and

$$|\tilde{\mathbb{E}}^N[g(i_1) \ldots g(i_k)] - (\tilde{\mathbb{E}}^N[g(1)])^k| \leq \Delta_N^{(k)} \qquad (10.13)$$

for all $1 \leq i_1 < i_2 < \ldots < i_k \leq N$

---

[18] This property can be recognized as an instance of the equivalence between microcanonical and canonical ensembles.

Then, one subsequently gets

$$
\begin{aligned}
\tilde{\mathbb{E}}^N[m^N(\eta_t)] &= \frac{1}{N}\sum_{i=1}^{N}\tilde{\mathbb{E}}^N[\eta_0(i-t)\{1-2g(i-t)\}\ldots\{1-2g(i-1)\}] \\
&= \tilde{\mathbb{E}}^N[\eta_0(1)]\,\tilde{\mathbb{E}}^N[\{1-2g(1)\}\ldots\{1-2g(t)\}] \\
&= m_0\{(1-2\,\tilde{\mathbb{E}}^N[g(1)])^t + A_N\} \\
&= m_0(1-2\rho)^t + o(1)
\end{aligned}
$$
(10.14)

by using that $|A_N| \le \Delta_N^{(t)}$ due to (10.13). Similarly for the second moment,

$$
\begin{aligned}
\tilde{\mathbb{E}}^N[(m^N(\eta_t))^2] &= \frac{1}{N}\sum_{i=1}^{N}\tilde{\mathbb{E}}^N[\eta_0(1)\,\eta_0(i)]\,\tilde{\mathbb{E}}^N[\{1-2g(1)\}\ldots\{1-2g(t)\} \\
&\qquad \times \{1-2g(i)\}\ldots\{1-2g(i+t-1)\}]
\end{aligned}
$$
(10.15)

Observe that for $t+1 \le i \le N+1-t$ there is no pair of the g's in the above product, acting on the same site. Hence, using the permutation-invariance and the asymptotic decoupling (10.12)–(10.13),

$$
\begin{aligned}
\tilde{\mathbb{E}}^N[(m^N(\eta_t))^2] &= \frac{1}{N}\sum_{i=t+1}^{N+1-t}\{m_0^2 + B_N(i)\}\{(1-2\,\tilde{\mathbb{E}}^N[g(1)])^{2t} + C_N(i)\} \\
&\quad + \frac{1}{N}\Big(\sum_{i=1}^{t}+\sum_{i=N+2-t}^{N}\Big)\{m_0^2 + B_N(i)\} \\
&\qquad \times \tilde{\mathbb{E}}^N[\{1-2g(1)\}\ldots\{1-2g(t)\} \\
&\qquad\quad \times \{1-2g(i)\}\ldots\{1-2g(i+t-1)\}] \\
&= \frac{N-2t+1}{N}m_0^2(1-2\rho)^{2t} + o(1) \\
&= m_0^2(1-2\rho)^{2t} + o(1)
\end{aligned}
$$
(10.16)

since the remainders satisfy $|B_N(i)| \le \Delta_N^{(2t)}$, $|C_N(i)| \le \Delta_N^{(2t)}$ for all i, and using a simple bound on the last term. The weak law of large numbers (10.7) then follows from (10.14) and (10.16) via a Chebyshev inequality.

Remark that there is a considerable freedom in the choice of the measures from which the initial configurations are sampled. The 'microcanonical' measure

$$
\tilde{\mathbb{P}}^N[\cdot] = \mathbb{P}^N[\cdot \mid m^N(\eta) = m_0;\ \rho^N(g) = \rho]
$$
(10.17)

is most natural but for obtaining (10.7), it can be replaced by various other ensembles. There is for example the 'canonical' measure

$$\mathbb{P}_{\text{can}}^N[(\eta, g)] = \frac{1}{\mathcal{Z}^N} \exp \sum_{i=1}^{N} (\beta\eta(i) + \alpha g(i)) \tag{10.18}$$

with the Lagrange multipliers β, α being fixed by the conditions

$$\mathbb{E}_{\text{can}}^N[\eta(1)] = m_0, \qquad \mathbb{E}_{\text{can}}^N[g(1)] = \rho$$

and $\mathcal{Z}^N$ is the normalization factor. It is easy to check that the autonomy (10.7) remains true if replacing $\tilde{\mathbb{P}}^N$ with $\mathbb{P}_{\text{can}}^N$; in fact, the proof is simpler now since $\mathbb{P}_{\text{can}}^N$ exactly factorizes and hence the above remainders A_N, B_N, C_N as in (10.14) and (10.16) are zero.
The corresponding large deviation rate function $s_{\text{can}}(\eta, g)$ which enters the law

$$\mathbb{P}_{\text{can}}^N[(m^N(\eta), \rho^N(g)) \simeq (m, \rho)] \simeq e^{N s_{\text{can}}(m, \rho)} \tag{10.19}$$

can also be computed (the easiest via the Gartner-Ellis theorem, [9]) with the result $s_{\text{can}}(m, \rho) = s(m, \rho)$. This equality shows the equivalence of ensembles on the level of entropies, which is well studied in equilibrium statistical physics. We come back to the problem of equivalence within a quantum framework and in a substantially larger generality in Section 13.4.

10.3. **Irreversibility and entropy production.** Consider a modification of the microdynamics (10.1) in which the particles jump to the left instead of to the right. It is given by the map

$$(\bar{U}(\eta, g))(i) = ([1 - 2g(i)]\, \eta(i + 1), \, g(i)) \quad \text{mod } N \tag{10.20}$$

which is an inverse of U, i.e., $\bar{U} \circ U = U \circ \bar{U} = 1$. The spin configuration at time t as evolved from η through the dynamics $\bar{U}$ is denoted by $\bar{\eta}_t$:

$$\bar{\eta}_t(i) = \eta_0(i + t)[1 - 2g(i + t - 1)] \ldots [1 - 2g(i)] \tag{10.21}$$

Observe that the sequence (trajectory) $(\eta_0, \eta_1, \ldots, \eta_t)$ is allowed (possible) under the original microscopic dynamics iff $(\eta_t, \eta_{t-1}, \ldots, \eta_0)$ is possible under U. That invertibility is referred to as *dynamical (time-)reversibility*. It can be formulated differently by extending the configuration space K with a 'velocity' variable $v \in \{-1, 1\}$ and by defining the dynamics via the transformation

$$V(\eta, g, v) = \begin{cases} (U(\eta, g), v) & \text{if } v = +1 \\ (\bar{U}(\eta, g), v) & \text{if } v = -1 \end{cases} \tag{10.22}$$

With the involution π, $\pi(\eta, g, v) = (\eta, g, -v)$ the dynamical reversibility gets the form: $\pi \circ V \circ \pi = V^{-1}$; the time-reversed microscopic dynamics is then achieved by inverting the velocity v.

The macroscopic time-evolution ϕ in which $m \mapsto (1-2\rho)m \in [-1, 1]$ is invertible as well (provided that $\rho \neq \frac{1}{2}$). Yet, the typical macroscopic time-evolution corresponding to $\bar{U}$ is not ϕ^{-1} but rather ϕ again, i.e., the law of large numbers (10.7) stays true when replacing U and η_t with $\bar{U}$ and $\bar{\eta}_t$! It simply means that the macroscopic evolution $m \mapsto m(1-2\rho)$ does *not* get inverted by starting from a *typical* microscopic configuration η corresponding to the macroscopic state $m(1-2\rho)$ and by applying the inverted microscopic dynamics (or by inverting the velocity). Naturally, there exist microscopic configurations η for which the inverted macroevolution $m(1 - 2\rho) \mapsto m$ along the dynamics $\bar{U}$ would be observed—this is precisely what the dynamical reversibility claims—they show up to be exceedingly *exceptional* under $m(1 - 2\rho)$, however. This physical impossibility to invert the macroscopic evolution is referred to as *macroscopic irreversibility.*

The macroscopic irreversibility in the above sense on the one hand and the strict increase of the Boltzmann entropy on the other hand, are often used as synonyms. Let us formulate their relation a bit more precisely. Observe that the two sets

$$\{(\eta_0, g) : m^N(\eta_0) \stackrel{\delta}{=} m_0; \ m^N(\eta_t) \stackrel{\delta}{=} m_t; \ \rho^N(g) \stackrel{\delta}{=} \rho\}$$

and

$$\{(\eta_0, g) : m^N(\bar{\eta}_t) \stackrel{\delta}{=} m_0; \ m^N(\eta_0) \stackrel{\delta}{=} m_t; \ \rho^N(g) \stackrel{\delta}{=} \rho\}$$

with $m_t = m_0(1 - 2\rho)^t$ have the same cardinalities (check that the map $\bar{U}$ is a bijection between these sets). Hence, they have the same measures under $\mathbb{P}^N$, which we write as

$$
\begin{aligned}
\log \mathbb{P}^N[m^N(\eta_t) &\stackrel{\delta}{=} m_t \mid m^N(\eta_0) \stackrel{\delta}{=} m_0; \ \rho^N(g) \stackrel{\delta}{=} \rho] \\
&+ \log \mathbb{P}^N[m^N(\eta_0) \stackrel{\delta}{=} m_0; \ \rho^N(g) \stackrel{\delta}{=} \rho] \\
= \log \mathbb{P}^N[m^N(\bar{\eta}_t) &\stackrel{\delta}{=} m_0 \mid m^N(\eta_0) \stackrel{\delta}{=} m_t; \ \rho^N(g) \stackrel{\delta}{=} \rho] \\
&+ \log \mathbb{P}^N[m^N(\eta_0) \stackrel{\delta}{=} m_t; \ \rho^N(g) \stackrel{\delta}{=} \rho]
\end{aligned}
\tag{10.23}
$$

Dividing by N, taking the limits $N \uparrow \infty$ and $\delta \downarrow 0$ in this order, and using the law of large numbers (10.7), we get the large deviation law

$$
\begin{aligned}
\lim_{\delta \downarrow 0} \lim_{N \uparrow \infty} \frac{1}{N} \log \mathbb{P}^N[m^N(\bar{\eta}_t) &\stackrel{\delta}{=} m_0 \mid m^N(\eta_0) \stackrel{\delta}{=} m_t; \ \rho^N(g) \stackrel{\delta}{=} \rho] \\
&= s(m_0, \rho) - s(m_t, \rho)
\end{aligned}
\tag{10.24}
$$

or

$$\mathbb{P}^N[m^N(\bar{\eta}_t) \simeq m_0 \mid m^N(\eta_0) \simeq m_t; \ \rho^N(g) \simeq \rho] \simeq e^{-N[s(m_t, \rho) - s(m_0, \rho)]} \tag{10.25}$$

which is quite a remarkable relation. Notice first that it provides another derivation of the H-theorem: since the left-hand side is less than one, one immediately gets $s(m_t, \rho) \geq s(m_0, \rho)$. Further, the left-hand

side is nothing but the probability that a configuration η_0 sampled from macrostate m_t and evolved according to $\bar{U}$, exhibits the macroscopic transition from m_t to m_0, which is just an inversion of the typical transition $m_0 \mapsto m_t$.

Macroscopic irreversibility amounts to the statement that such inverted macroscopic transitions are physically impossible; here we have a quantitative evaluation how rare they really are: the large deviation rate function for the backward transition $m_t \mapsto m_0$ with respect to $\bar{U}$ just coincides with the entropy production along the *typical* macroevolution $m_0 \mapsto m_t$ with respect to microscopic dynamics U. Inverting the logic, this can be read off as a formula for the entropy production, possibly useful provided that the probability of those rare backward transitions can be evaluated or estimated.

The seeming inconsistency between the microscopic reversibility and the macroscopic irreversibility is known as the Loschmidt paradox. Equality (10.25) in a sense solves this paradox and put it in a correct perspective: those macroscopic trajectories obtained by time-reverting the typical ones $(\phi^t(m);\ t = 0, 1, \ldots)$ are indeed observable for finite N, however they are exponentially damped. Notice that (10.25) is nothing but a macroscopic analogue of the detailed balance condition (4.4) that we have already discussed in the context of lattice gases.

11. INFINITE SYSTEMS

The above analysis of the Kac model shows up to be quite generic and one can easily extend those arguments to a more general setup. The aim of the present section is to formulate general sufficient conditions for the existence of a Lyapunov function for a class of macroscopic dynamics, or, equivalently, for an H-theorem to be valid.

11.1. Dynamical systems, macrostates, and entropy. On a microscopic level, we consider a family of classical dynamical systems $(K^N, U_t^N, \mathbb{P}^N)_{N \uparrow +\infty}$, where the label N should be thought of as a spatial extension of the system and the maps[19] $(U_t^N)_{t \geq 0}$ are assumed to satisfy the semigroup condition $U_t^N U_s^N = U_{t+s}$ for all $t, s \geq 0$. The probability measures $\mathbb{P}^N$ are invariant under the dynamics: $\mathbb{P}^N(U^N)^{-1} = \mathbb{P}^N$.

The macroscopic level of description is specified by a collection of macroscopic observables. These are some maps $M^N : K^N \mapsto \Omega$ into a metric space (Ω, d) of *macrostates*. We assign to every $m \in \Omega$ the

---

[19]Depending on an application, the maps U_t^N can be e.g. Hamiltonian flows, possibly with the time and space suitably rescaled with N. The details are not really important for what follows, we will only require the microscopic dynamics to satisfy a few general conditions, see below.

Boltzmann entropy defined as the large deviation rate function under the measures $\mathbb{P}^N$:

$$s(m) = \lim_{\delta \downarrow 0} \limsup_{N \uparrow +\infty} \frac{1}{N} \log \mathbb{P}^N[M^N(x) \overset{\delta}{=} m], \qquad m \in \Omega \qquad (11.1)$$

using the shorthand $m \overset{\delta}{=} m'$ whenever $d(m, m') \leq \delta$. Denote

$$\Omega_0 = \{m \in \Omega;\ s(m) > -\infty\} \qquad (11.2)$$

the set of those macrostates that are admissible; we assume $\Omega_0 \neq \emptyset$. Note this is a first nontrivial assumption: the parametrization by N and an eventual rescaling have to be meaningful so that (M^N) indeed satisfies the large deviation principle with a finite rate function $s(m)$ on some large enough space Ω_0.

11.2. **Autonomous evolution and H-theorem.** Starting from a microscopic configuration $x \in K^N$, the macroscopic trajectory is simply the collection $(M^N(U_t^N x))_{t \geq 0}$. We assume the existence of an *autonomous* macroscopic dynamics in the following sense: let there be a collection $(\phi_t)_{t \geq 0}$ of maps $\phi : \Omega_0 \mapsto \Omega_0$ satisfying

(1) the semigroup condition

$$\phi_t \circ \phi_s = \phi_{t+s}, \qquad t, s \geq 0 \qquad (11.3)$$

(2) a weak autonomy condition

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \mathbb{P}^N[M^N(U_t^N x) \overset{\delta}{=} \phi_t(m) \,|\, M^N(x) \overset{\delta}{=} m] = 0 \qquad (11.4)$$

for all $t \geq 0$ and $m \in \Omega_0$.

Notice that (11.4) is a much weaker condition than the law of large numbers (10.7) valid for the Kac model. In particular, no typical macroscopic evolution is required to exist; that $(\phi_t)_{t \geq 0}$ can e.g. be a single realization of a stochastic process describing a macroscopic evolution of a system passing through a number of branching points.[20] On the other hand, this condition is generally not satisfied by stochastic systems on mesoscopic scale and/or without involving the large N limit. In that sense, condition (11.4) draws a sharp border line between macroscopic and mesoscopic systems.

Since $\mathbb{P}^N$ is invariant under U_t^N, conditions (11.3)–(11.4) are equivalent with a single condition

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \mathbb{P}^N[M^N(U_t^N x) \overset{\delta}{=} \phi_t(m) \,|\, M^N(U_s x) \overset{\delta}{=} \phi_s(m)] = 0$$

$$(11.5)$$

---

[20]To have in mind a specific scenario, think of a ferromagnet being cooled down from a high-temperature paramagnetic state. When passing the critical temperature, the system randomly (= depending on the initial microscopic configuration) chooses one of the ferromagnetic states with broken symmetry.

required for all $t \geq s \geq 0$. Using the invariance $\mathbb{P}^N$ again, we find that for any pair $m, m' \in \Omega_0$ of macrostates,

$$
\begin{aligned}
\log \mathbb{P}^N(M^N(x) \overset{\delta}{=} m') &= \log \mathbb{P}^N(M^N(U_t^N x) \overset{\delta}{=} m') \\
&\geq \log \mathbb{P}^N(M^N(U_t^N x) \overset{\delta}{=} m' \mid M^N(U_s^N x) \overset{\delta}{=} m) \\
&\quad + \log \mathbb{P}^N(M^N(U_s^N x) \overset{\delta}{=} m)
\end{aligned}
\tag{11.6}
$$

which we are again going to divide by N, to take the upper limit $N \uparrow +\infty$ and then to take the limit $\delta \downarrow 0$. Choosing first $m = \phi_s(m)$ and $m' = \phi_t(m)$, autonomy condition (11.5) yields

$$
s(\phi_t(m)) \geq s(\phi_s(m)), \qquad t \geq s \geq 0 \tag{11.7}
$$

which is an H-theorem. Second, for $m = \phi_t(m)$ and $m' = \phi_s(m)$ it yields the inequality

$$
- \lim_{\delta \downarrow 0} \limsup_{N \uparrow +\infty} \frac{1}{N} \log \mathbb{P}^N(M^N(U_t^N x) \overset{\delta}{=} \phi_s(m) \mid M^N(U_s^N x) \overset{\delta}{=} \phi_t(m))
$$
$$
\geq s(\phi_t(m)) - s(\phi_s(m)) \quad (11.8)
$$

again for all $t \geq s \geq 0$, which provides an upper bound on the Boltzmann entropy production.

For an invertible microdynamics (U_t^N) inequalities (11.7)–(11.8) can be turned into a single equality by essentially repeating the computation of Section 10.3, see (10.23)–(10.24). The result reads

$$
s(\phi_t(m)) - s(\phi_s(m)) = \bar{J}_{s,t}(\phi_t(m), \phi_s(m)) \geq 0 \tag{11.9}
$$

where

$$
-\bar{J}_{s,t}(m, m')
$$
$$
= \lim_{\delta \downarrow 0} \limsup_{N \uparrow +\infty} \frac{1}{N} \log \mathbb{P}^N[M^N(\bar{U}_t^N x) \overset{\delta}{=} m' \mid M^N(\bar{U}_s^N x) \overset{\delta}{=} m] \quad (11.10)
$$

is the rate function for the transition from macrostate m at time s to macrostate m' at time t along the time-reversed dynamics $\bar{U}_t^N \equiv (U_t^N)^{-1}$. The conclusions of Section 10.3 apply as well in this general case: $\bar{J}_{s,t}(\phi_t(m), \phi_s(m))$ is a natural 'measure' of macroscopic irreversibility, and we have proven it is just equal to the entropy production for the transition $\phi_s(m) \mapsto \phi_t(m)$ fulfilling the autonomy (11.5).

Semigroup condition (11.3) is crucial and cannot be simply relaxed. Indeed, assuming only the autonomy in the form (11.4), one would still have the inequality between the initial and final Boltzmann entropies: $s(\phi_t(m)) \geq s(m)$, $t \geq 0$, however, $s(m_t)$ might not be monotone in general. As an example, think of the macrodynamics $\phi_t : \mathbb{R} \mapsto \mathbb{R}$

given as $\phi_t(m) = m\, r^t \cos \omega t$, $|r| < 1$, which is like the position of an underdamped pendulum swinging around its equilibrium position.

The missing semigroup property can be recovered by including additional macroscopic observables; in the case of the pendulum one would naturally add its velocity as another observable. To conclude, the semigroup condition is basically a restriction on the choice of the collection of macroscopic observables, which needs to be in that sense 'complete.'

12. FINITE SYSTEMS

In this section we evaluate the necessity of the large N limit in the above arguments, and we attempt a microscopic formulation of the H-theorem for an entropy defined upon a finite system and as a functional on microscopic configurations.

12.1. **Zermelo-Poincaré paradox.** For any fixed N the dynamical system $(K, U_t, \mathbb{P}) \equiv (K^N, U_t^N, \mathbb{P}^N)$ is really a *finite size* system; this is encoded by the assumption that $\mathbb{P}$ is a probability (and hence normalizable) measure. For simplicity, we consider in this section a macroscopic observable $M : K \mapsto \Omega$ such that

$$\Omega_0 = \{m \in \Omega; \ \mathbb{P}[M^{-1}(m)] > 0\} \qquad (12.1)$$

is finite or countable. As entropy function we take

$$S(m) = \log \mathbb{P}[M^{-1}(m)], \qquad m \in \Omega_0 \qquad (12.2)$$

The well-known Poincaré recurrence theorem then reads that for $\mathbb{P}$−almost every microstate $x \in K$ and any time t_0 one has $M(U_t x) = M(x)$ for some $t > t_0$, i.e., the trajectory almost surely returns back to the initial macrostate $M(x)$. This is usually phrased as the impossibility for the entropy (12.10) to be an increasing (nonconstant) function of time, which is also known as the Zermelo(-Poincaré) paradox. However, the analysis in the previous section and the Kac example give a clue: the recurrence time increases with the system size N and is shifted away to infinity in the thermodynamic limit.[21]

In the context of H-theorems it is instructive to reformulate Zermelo's objection in still a slightly modified way. There is in fact a tempting 'trivialization' of the argument leading to the H-theorem which goes as follows:

For our finite system, the autonomy could simply mean that the macroscopic evolution as specified by a map $\phi : \Omega_0 \mapsto \Omega_0$ is just what takes place for almost every microstate, i.e., that for $\mathbb{P}$−a.e. $x \in K$ one has

$$M(U_t x) = \phi_t(M(x)), \qquad t \geq 0 \qquad (12.3)$$

---

[21]For the Kac example the recurrence time is of order N. However, in many dynamical systems it goes exponentially with the number of degrees of freedom, which is itself $e^{O(N)}$.

Were this indeed true as such, it would automatically imply the semigroup condition since, almost surely,

$$M(U_{t+s}x) = \phi_t(M(U_s x)) = \phi_t \circ \phi_s(M(x)), \qquad t, s \geq 0 \qquad (12.4)$$

Second, it would mean that

$$\mathbb{P}[(U_t)^{-1} M^{-1}(m_t) \cap M^{-1}(m)] = \mathbb{P}[M^{-1}(m)] \qquad (12.5)$$

with $m_t = \phi_t(m)$, i.e., the set of microstates $M^{-1}(m)$ evolves to a subset of $M^{-1}(m_t)$, up to a zero measure set. Hence,

$$S(m_t) = \log \mathbb{P}[(U_t)^{-1} M^{-1}(m_t)] \geq \mathbb{P}[M^{-1}(m)] = S(m) \qquad (12.6)$$

due to the invariance of $\mathbb{P}$. Finally,

$$S(m_t) = S(\phi_{t-s}(m_s)) \geq S(m_s), \qquad t \geq s \geq 0 \qquad (12.7)$$

On the other hand, by the above Poincaré recurrence, $S(m_t) = S(m)$ for infinitely many t, and hence $S(m_t)$ is constant!

The above computation shows that the assumption of autonomy in the form (12.3) or (12.5) is too strong. If fulfilled, the macroscopic evolution would necessarily be reversible and the entropy constant. Our condition of autonomy (11.4) is much weaker and it does not guarantee the semigroup property. In the Kac example, the law of large number (10.7) is far stronger than autonomy (11.4), yet still consistent with a macroscopic irreversible evolution, as we have checked explicitly.

12.2. **Microscopic H-theorem.** We come back to the general framework of Section 11.1 and consider again a sequence of dynamical systems $(K^N, U_t^N, \mathbb{P}^N)_N$ and a general macroscopic observable $M^N : K^N \to \Omega$, macroscopic in the sense that Ω_0 defined in (11.1) is nonempty. Our aim is now to formulate an H-theorem for Boltzmann entropy assigned to each *microstate* of a single, possibly large finite-size system. Put it differently, we want to see how much the entropy is allowed to fluctuate around a monotone path when evaluated along a single microscopic trajectory of a single dynamical system with N large but fixed.

For N fixed the Boltzmann entropy is no longer unambiguously defined since the sets $\{x; \ M^N(x) \overset{\delta}{=} m\}$ depend on the width $\delta > 0$ and are not necessarily all disjoint for different macroscopic states m. To be safe we assign to every microstate $x \in K^N$ the interval $[S_<^{N,\delta}(x), S_>^{N,\delta}(x)]$ of entropies defined as

$$S_<^{N,\delta}(x) = \inf_{m \in \Omega_0} \{S^{N,\delta}(m); \ m \overset{\delta}{=} M^N(x)\} \qquad (12.8)$$

$$S_>^{N,\delta}(x) = \sup_{m \in \Omega_0} \{S^{N,\delta}(m); \ m \overset{\delta}{=} M^N(x)\} \qquad (12.9)$$

where

$$S^{N,\delta}(m) = \log \mathbb{P}^N[M^N(x) \overset{\delta}{=} m] \qquad (12.10)$$

We impose the autonomy assumption in the form of a law of large numbers:

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \mathbb{P}^N[M^N(U_t^N x) \stackrel{\delta}{=} \phi_t(m) \mid M^N(x) \stackrel{\delta}{=} m] = 1 \qquad (12.11)$$

for all $m \in \Omega_0$, $t \geq 0$, and with maps $\phi_t : \Omega_0 \mapsto \Omega_0$ such that $\phi_t \circ \phi_s = \phi_{t+s}$, $t \geq s \geq 0$.

Let us fix some initial condition $m \in \Omega_0$, $\delta > 0$ and a finite sequence of times $0 = t_0 < t_1 < \ldots < t_Q$. Combining assumption (12.11) with the semigroup condition, the remainder

$$D^{N,\delta}(s,t;m) := 1 - \mathbb{P}^N[M^N(U_t^N x) \stackrel{\delta}{=} \phi_t(m) \mid M^N(U_s^N x) \stackrel{\delta}{=} \phi_s(m)] \tag{12.12}$$

satisfies $\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} D^{N,\delta}(s,t;m) = 0$ whenever $t \geq s \geq 0$. By subadditivity,

$$\mathbb{P}^N[M^N(U_{t_j}^N x) \stackrel{\delta}{=} \phi_{t_j}(m),\ j = 1,\ldots,Q \mid M^N(x) \stackrel{\delta}{=} m]$$
$$\geq 1 - \sum_{j=1}^{Q} D^{N,\delta}(0,t_j;m) \quad (12.13)$$

Whenever $m^N(U_t x) \stackrel{\delta}{=} \phi_t(m)$ then

$$S_<^{N,\delta}(U_t^N x) \leq S^{N,\delta}(\phi_t(m)) \leq S_>^{N,\delta}(U_t^N x) \qquad (12.14)$$

As a consequence, (12.13) gives

$$\mathbb{P}^N[S_<^{N,\delta}(U_{t_j} x) \leq S^{N,\delta}(\phi_{t_j}(m)) \leq S_>^{N,\delta}(U_{t_j} x),\ j = 1,\ldots,Q \mid M^N(x) \stackrel{\delta}{=} m]$$
$$\geq 1 - \sum_{j=1}^{Q} D^{N,\delta}(0,t_j;m) \quad (12.15)$$

Entropies at successive times satisfy the inequality following from (12.12):

$$S^{N,\delta}(\phi_{t_j}(m)) \geq S^{N,\delta}(\phi_{t_{j-1}}(m)) + \log(1 - D^{N,\delta}(t_{j-1},t_j;m)) \quad (12.16)$$

Using that

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \min_{j=1}^{Q} \log(1 - D^{N,\delta}(t_{j-1},t_j;m)) = 0 \qquad (12.17)$$

inequalities (12.15)–(12.16) yield the main result of this section:

For any $\Delta > 0$, $m \in \Omega_0$, and a finite sequence $0 = t_0 < t_1 < \ldots t_Q$ of times, one has

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \mathbb{P}^N[S_>^{N,\delta}(U_{t_j} x) \geq S_<^{N,\delta}(U_{t_{j-1}} x) - \Delta,\ j = 1,\ldots,Q \mid M^N(x) \stackrel{\delta}{=} m] = 1$$
$$(12.18)$$

Therefore, the finite-system entropy violates the monotonicity as little as required with probability arbitrarily closed to one, provided that δ is small enough and N large enough. This is the announced microscopic

H-theorem.

Remark that the ambiguity with the definition of finite-system entropy does not arise if the observables M^N take only finitely or countably many values (as in Section 12.1 but this time uniformly for all N). In that case, one can set $\delta = 0$ and the entropy is simply

$$S^N(x) := S_<^{N,0}(x) = S_>^{N,0}(x) = \log \mathbb{P}^N[(M^N)^{-1}M^N(x)] \qquad (12.19)$$

(Compare with (12.2).) The microscopic H-theorem (12.18) then becomes, under the same assumptions,

$$\lim_{N\uparrow+\infty} \mathbb{P}^N[S^N(U_{t_j}x) \geq S^N(U_{t_{j-1}}x) - \Delta, \; j = 1, \ldots, Q \,|\, M^N(x) = m] = 1 \qquad (12.20)$$

13. QUANTUM SYSTEMS

The arguments presented in the previous section do not dramatically change when passing from a classical to a quantum dynamics. What does need to be refined however, is the very description of macroscopic states due to the inherent incompatibility of quantum observables, as visible from the noncommutativity of corresponding (self-adjoint) operators before any macroscopic limit is taken.

Obviously, the question of a quantum fluctuation theory and of quantum limiting behavior is not restricted to nonequilibrium physics. The difference between equilibrium and nonequilibrium macroscopic states lies mainly in the choice of macroscopic constraints. The constraints describing equilibrium (like energy, particle number) usually commute and hence the problem we discuss here typically falls in a nonequilibrium context.

A first attack on this problem dates back to John von Neumann, [46]. His idea went as follows: The single particle position and momentum operators Q, P satisfy the commutation relation[22] $[Q, P] = i$. Hence, assigning copies Q_i, P_i, $i = 1, \ldots, N$ to each of N particles, the averages $Q^N = \frac{1}{N}\sum_i Q_i$, $P^N = \frac{1}{N}\sum_i P_i$ satisfy $[Q^N, P^N] = \frac{i}{N}$. Although they do not commute and hence cannot be diagonalized together (nor simultaneously measured), one can think of suitable modifications $\tilde{Q}^N$, $\tilde{P}^N$ that already commute and that in a sense well approximate the originals, at least for large N. Indeed, von Neumann explicitly constructs commuting operators $\tilde{Q}^N$, $\tilde{P}^N$ which have purely discrete spectra of nondegenerate eigenvalues $(q_\alpha^N, p_\alpha^N)_\alpha$, and whose eigenvectors $(\psi_\alpha^N)_\alpha$ make a complete orthonormal basis system in $L^2(\mathbb{R})$. They approximate the operators Q^N, P^N in the sense that

$$(\psi_\alpha^N, Q^N\psi_\alpha^N) = q_\alpha^N, \qquad (\psi_\alpha^N, P^N\psi_\alpha^N) = p_\alpha^N \qquad (13.1)$$

---

[22]Set the Planck constant to one.

and

$$\|(Q^N - q_\alpha^N)\,\psi_\alpha^N\| \leq \frac{C}{\sqrt{N}}\,, \qquad \|(P^N - p_\alpha^N)\,\psi_\alpha^N\| \leq \frac{C}{\sqrt{N}} \qquad (13.2)$$

with $C \approx 60$, see [46] for details.

What follows is a slight modification and generalization of the above idea that comes close to the point of view of quantum information theory. Instead of modifying the operators themselves, we look for the largest or typical subspaces that in some sense well approximate the eigenspaces for given eigenvalues, simultaneously for *all* macroscopic observables from a collection. This construction proves to be natural since the corresponding entropy, measuring the dimension of that typical subspace, actually satisfies a variational principle. Hence, it can be directly compared with another, more familiar although physically less satisfactory construction based on maximizing the von Neumann entropy. The (non)equality of both entropies is then a problem of (non)equivalence of ensembles. Looked at from another angle, such an equivalence gives a counting interpretation to the von Neumann entropy in the thermodynamic limit, and opens interesting possibilities towards a consistent and meaningful scheme of quantum large deviations.

13.1. **Quantum macrostates and entropy.** A macroscopically large quantum system is modeled by a sequence of finite-dimensional Hilbert spaces $(\mathcal{H}^N)_{N\uparrow+\infty}$ on which we have standard traces Tr^N. As macroscopic observables we consider a collection $M^N = (M_k^N)_{k\in I}$ of self-adjoint operators on $\mathcal{H}^N$; for simplicity, we assume I to be finite. For each operator there is a projection-valued measure $\mathcal{Q}_k^N$ on $\mathbb{R}$ such that, by the spectral theorem,

$$F(M_k^N) = \int_{\mathbb{R}} \mathcal{Q}_k^N(\mathrm{d}z)\,F(z)\,, \qquad F \in C(\mathbb{R}) \qquad (13.3)$$

(which is just to say that M_k^N is unitarily equivalent to a multiplication, or simply that M_k^N can be diagonalized.) A quantum counterpart of the classical set of microstates $M_k^N \overset{\delta}{=} m_k$ for some macrostate $m_k \in \mathbb{R}$ is the projection

$$\mathcal{Q}_k^{N,\delta}(m_k) = \int_{m_k-\delta}^{m_k+\delta} \mathcal{Q}_k^N(\mathrm{d}z) \qquad (13.4)$$

13.1.1. *Commuting observables.* As a warm-up, assume first that M^N is a collection of mutually commuting operators. In that case, $\mathcal{Q}^N(\mathrm{d}z) = \prod_{k\in I} \mathcal{Q}_k^N(\mathrm{d}z_k)$ is a common projection-valued measure, (13.3) extends to

$$F(M^N) = \int_{\mathbb{R}^I} \mathcal{Q}^N(\mathrm{d}z)\,F(z)\,, \qquad F \in C(\mathbb{R}^I) \qquad (13.5)$$

and a macrostate $m = (m_k)_{k \in I}$ gets represented by the projection

$$\mathcal{Q}^{N,\delta}(m) = \prod_{k \in I} \mathcal{Q}_k^{N,\delta}(m_k) \tag{13.6}$$

The classical entropy, say in the form (12.10), extends to

$$S^{N,\delta}(m) = \log \mathrm{Tr}^N[\mathcal{Q}^{N,\delta}(m)] \tag{13.7}$$

This is a formalism entirely equivalent to the one for classical systems.

13.1.2. *General observables.* For a general collection M^N of observables and a macrostate $m \in \mathbb{R}^I$, projections $(\mathcal{P}^N)_{N\uparrow+\infty}$ are said to be *concentrating* at m, written $\mathcal{P}^N \to m$, whenever

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N[F(M_k^N) \,|\, \mathcal{P}^N] = F(m_k) \tag{13.8}$$

is satisfied for all $F \in C(\mathbb{R})$ and $k \in I$, with the notation

$$\mathrm{tr}^N[\,\cdot\,|\,\mathcal{P}^N] = \frac{\mathrm{Tr}^N[\mathcal{P}^N \cdot\,]}{\mathrm{Tr}^N[\mathcal{P}^N]} \tag{13.9}$$

for the normalized trace on $\mathcal{P}^N \mathcal{H}^N$. Condition (13.8) is a law of large numbers for observables M_k^N under quantum state (13.9); it can be equivalently written as the condition

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N[\mathcal{Q}_k^{N,\delta}(m_k) \,|\, \mathcal{P}^N] = 1 \tag{13.10}$$

for any $\delta > 0$ and $k \in I$. Physically, it means that all M_k^N, $k \in I$ are asymptotically dispersionless under state (13.9).

Having in mind the classical situation where the entropy counts the number of *all* microstates x such that $M^N(x) \overset{\delta}{=} m$, we are mostly interested in those concentrating sequences that are maximal in the sense of dimension counting. Hence, we define the (infinite-system, Boltzmann) entropy $s(m)$ for any $m = (m_k)_{k \in I}$ by the variational problem

$$s(m) = \limsup_{\mathcal{P}^N \to m} \frac{1}{N} \log \mathrm{Tr}^N[\mathcal{P}^N] \tag{13.11}$$

i.e., $s(m)$ is the largest limit point over all projections concentrating at m. Any projections $\mathcal{P}^N$ attaining the entropy $s(m)$ in the large N limit,

$$\limsup_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[\mathcal{P}^N] = s(m) \tag{13.12}$$

are then called *typical* projections concentrating at m.[23] Clearly, they provide a variant of the microcanonical ensemble for noncommuting observables. An example comes in Section 14.

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[23]Note a slight difference in the terminology with respect to [12] where the typical concentrating projections were rather called a microcanonical macrostate. The present terminology is closer to the one of quantum information theory.

To check that the above definition of entropy is meaningful, we first revisit the relation between the macroscopic autonomy and the H-theorem of Section 12.2 in the present quantum set-up. Second, we link our construction to the canonical construction based on maximizing the von Neumann entropy, and we prove that they are equivalent under suitable conditions.

13.2. **H-theorem.** As a microscopic dynamics we consider a family of automorphisms[24] $(\tau_t^N)_{t \geq 0}$ acting on the observables from $\mathcal{B}(\mathcal{H}^N)$ and having the semigroup property

$$\tau_t^N \tau_s^N = \tau_{t+s}^N, \qquad t, s \geq 0 \tag{13.13}$$

Denote

$$\Omega_0 = \{m \in \mathbb{R}^I; \, s(m) \geq 0\} \tag{13.14}$$

the set of all admissible macrostates. The conditions on the emergent macroscopic dynamics now have the following form, cf. Section 12.2. There are maps $(\phi_t)_{t \geq 0}$ on Ω_0 satisfying

(1) *semigroup condition*: $\phi_t \circ \phi_s = \phi_{t+s}$, $t, s \geq 0$;
(2) *autonomy condition*: for every $m \in \Omega_0$ there exist some typical projections $\mathcal{P}^N \to m$ concentrating at m such that for all $F \in C(\mathbb{R})$, $k \in I$, and $t \geq 0$,

$$\lim_{N \uparrow +\infty} \mathrm{tr}^N[\tau_t^N F(M_k^N) \,|\, \mathcal{P}^N] = F((\phi_t m)_k) \tag{13.15}$$

or, equivalently,

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \mathrm{tr}^N[\tau_t^N \mathcal{Q}_k^{N,\delta}((\phi_t m)_k) \,|\, \mathcal{P}^N] = 1 \tag{13.16}$$

Under these condition it is easy to prove that

$$s(\phi_t m) \geq s(\phi_s m), \qquad m \in \Omega_0, \, t \geq s \geq 0 \tag{13.17}$$

Indeed, let $\mathcal{P}^N \to m$ be typical projections concentrating at m and verifying (13.15) or (13.16). Using that τ_t^N is invertible and $(\tau_t^N)^{-1}$ is again an automorphism such that $\mathrm{Tr}^N((\tau_t^N)^{-1}\cdot) = \mathrm{Tr}^N(\cdot)$, one has

$$\begin{aligned} \mathrm{tr}^N[\tau_t^N F(M_k^N) \,|\, \mathcal{P}^N] &= \frac{\mathrm{tr}^N[F(M_k^N)\,(\tau_t^N)^{-1}\mathcal{P}^N]}{\mathrm{tr}^N[(\tau_t^N)^{-1}\mathcal{P}^N]} \\ &= \mathrm{tr}^N[F(M_k^N) \,|\, (\tau_t^N)^{-1}\mathcal{P}^N] \end{aligned} \tag{13.18}$$

---

[24]This means that $\tau_t^N(XY) = \tau_t^N(X)\,\tau^N(Y)$ for any $X, Y \in \mathcal{B}(\mathcal{H}^N)$, which is a noncommutative generalization of classical deterministic map. Physically, $(\mathcal{H}^N, \tau_t^N, \mathrm{Tr}^N)$ models a *closed* quantum dynamical system; note that $\mathrm{Tr}^N(\tau_t^N(\cdot)) = \mathrm{Tr}^N(\cdot)$ and hence Tr^N corresponds to the invariant (counting, unnormalized) classical measure.

Hence, autonomy (13.15) implies that $(\tau_t^N)^{-1}\mathcal{P}^N$ concentrate at $\phi_t m$, $(\tau_t^N)^{-1}\mathcal{P}^N \to \phi_t m$.[25] As a result,

$$s(m) = \limsup_{N\uparrow+\infty} \frac{1}{N}\log \operatorname{Tr}^N[(\tau_t^N)^{-1}\mathcal{P}^N] \leq s(\phi_t m) \qquad (13.19)$$

By combining with the semigroup property,

$$s(\phi_t m) = s(\phi_{t-s}\circ\phi_s m) \geq s(\phi_s m) \qquad (13.20)$$

as claimed.

Notice that in (13.15)–(13.16) we have required the autonomy condition in the sense of a law of large numbers; compare with a much weaker assumption (11.4). A possible way how to prove the H-theorem under a weaker autonomy condition here too, might be via suitably weakening the notion of concentration and by modifying the definition of entropy; we do not discuss this issue.

13.3. **Canonical formalism.** Von Neumann has introduced the entropy functional on states $\omega^N(\cdot) = \operatorname{Tr}^N[\rho^N\cdot]$ over $\mathcal{B}(\mathcal{H}^N)$ by

$$\mathfrak{S}(\omega^N) = -\operatorname{Tr}^N[\rho^N\log\rho^N] \qquad (13.21)$$

For trace states on subspaces of $\mathcal{H}^N$, given as $\omega_{\mathcal{P}^N}^N(\cdot) = \operatorname{Tr}^N[\mathcal{P}^N\cdot]/\operatorname{Tr}^N[\mathcal{P}^N]$, the von Neumann entropy boils down to

$$\mathfrak{S}(\omega_{\mathcal{P}^N}^N) = \log\operatorname{Tr}^N[\mathcal{P}^N] \qquad (13.22)$$

In this light, entropy (13.11) can also be written as

$$s(m) = \limsup_{\mathcal{P}^N\to m} \frac{\mathfrak{S}(\omega_{\mathcal{P}^N}^N)}{N} \qquad (13.23)$$

A general and very successful approach in statistical physics lies in the idea that a variational principle like (13.23) can often be extended to a larger 'test space', so that (1) a new variational problem becomes easier to solve, and (2) the resulting entropy $s(m)$ can be proven to remain unchanged. This is a standard approach at least when describing thermal equilibrium, but it is often used in a similar way to describe nonequilibrium macroscopic states (sometimes then referred to as *constrained* equilibria).

To obtain the *canonical* description for a given macrostate $m \in \mathbb{R}^I$, we write $\omega^N \xrightarrow{1} m$ for any sequence of states satisfying $\lim_{N\uparrow+\infty}\omega^N(M_k^N) = m_k$, $k \in I$ (convergence in mean). Analogous to (13.23), we define the *canonical* entropy,

$$s_{\mathrm{can}}(m) = \limsup_{\omega^N\xrightarrow{1}m} \frac{\mathfrak{S}(\omega^N)}{N} \qquad (13.24)$$

---

[25]Note they do not have to be *typical* concentrating projections at $\phi_t m$!

Any sequence of states $(\omega^N)_{N\uparrow+\infty}$ such that $\lim_{N\uparrow+\infty} \mathfrak{S}(\omega^N)/N = s_{\mathrm{can}}(m)$ we then call *canonical states* at m.

An advantage of this formulation is that one can often find canonical states explicitly in a Gibbsian form: consider states $\omega_\lambda^N(\cdot) = \mathrm{Tr}^N[\rho_\lambda^N \cdot]$ defined as

$$\rho_\lambda^N = \frac{1}{\mathcal{Z}_\lambda^N} e^{N \sum_k \lambda_k M_k^N}, \qquad \mathcal{Z}_\lambda^N = \mathrm{Tr}^N[e^{N \sum_k \lambda_k M_k^N}] \qquad (13.25)$$

with some $\lambda = (\lambda_k)_{k \in I}$. If $\lim_{N\uparrow+\infty} \omega_\lambda^N(M_k^N) = m_k$, $k \in I$, then $(\omega_\lambda^N)_{N\uparrow+\infty}$ are canonical states at m.

This easily follows from the positivity of relative entropy, see e.g. [5]: for any $\omega^N \xrightarrow{1} m$, $\omega^N(\cdot) = \mathrm{Tr}^N[\rho^N \cdot]$,

$$\limsup_{N\uparrow+\infty} -\frac{1}{N} \omega^N[\log \rho^N] \leq \limsup_{N\uparrow+\infty} -\frac{1}{N} \omega^N[\log \rho_\lambda^N]$$

$$= \limsup_{N\uparrow+\infty} \frac{1}{N} \log \mathcal{Z}_\lambda^N - \sum_k \lambda_k m_k \qquad (13.26)$$

$$= \limsup_{N\uparrow+\infty} -\frac{1}{N} \omega_\lambda^N[\log \rho_\lambda^N]$$

as claimed. It also yields the canonical entropy in the form

$$s_{\mathrm{can}}(m) = p(\lambda) - \sum_k \lambda_k m_k \qquad (13.27)$$

where we have defined the 'pressure'

$$p(\lambda) = \limsup_{N\uparrow+\infty} \frac{1}{N} \log \mathcal{Z}_\lambda^N \qquad (13.28)$$

13.4. **Macroscopic equivalence.** By construction, $s_{\mathrm{can}}(m) \geq s(m)$. A natural question arises under what conditions both entropies are actually equal. This is a familiar problem of the equivalence of ensembles (microcanonical versus canonical in this case) on the level of entropies, however, the usual arguments, e.g. [37, 51, 19], are mostly restricted to the case of equilibrium and commuting observables (with the energy and/or the particle number as the only variables). The generalized microcanonical ensemble in the sense of Section 13.1.2 requires some refinement of those arguments. Below we provide some sufficient conditions for the equivalence.

Let $(\omega_\lambda^N)_{N\uparrow+\infty}$ be canonical states (13.25) with $\omega_\lambda^N \xrightarrow{1} m$. Assume that

(1) the limit

$$p(\lambda) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[e^{N \sum_k \lambda_k M_k^N}] \qquad (13.29)$$

exists and has the derivative $\frac{\mathrm{d}p(\kappa\lambda)}{\mathrm{d}\kappa}\big|_{\kappa=1} = \sum_k \lambda_k\, m_k$;

(2) for any $j \in I$, the generating function

$$q_j(\kappa) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[e^{N\sum_k \lambda_k M_k^N} e^{\kappa N M_j^N}] \tag{13.30}$$

exists and has the derivative $\frac{\mathrm{d}q_j(\kappa)}{\mathrm{d}\kappa}\big|_{\kappa=0} = m_j$.

Under these hypotheses we will prove that

$$s(m) = s_{\mathrm{can}}(m) = \sum_{k\in I} \lambda_k m_k - p(\lambda) \tag{13.31}$$

Remark that by the Golden-Thompson inequality,[26]

$$q_j(\kappa) \geq p(\lambda + (0, \ldots, (\kappa)_j, \ldots, 0)) \tag{13.32}$$

Unless M_N^k all mutually commute, this inequality generically becomes strict and those $(q_j)_{j\in I}$ are fundamentally different from the pressure; they appear naturally when studying quantum large fluctuations, see Section 13.5.

The proof of equivalence (13.31) comes in a sequence of steps: first we show that the canonical states ω_λ^N are exponentially concentrating at m, then we construct typical projections for these states, and finally we prove that those typical projections concentrate at m too.

13.4.1. *Exponential concentration.* By assumption, q_j exists in some interval $[-\kappa_0, \kappa_0]$, $\kappa_0 > 0$. From the spectral theorem (13.3),

$$\begin{aligned}
q_j(\kappa) &= p(\lambda) + \lim_{N\uparrow+\infty} \frac{1}{N} \log \omega_\lambda^N[e^{\kappa N M_j^N}] \\
&= p(\lambda) + \lim_{N\uparrow+\infty} \frac{1}{N} \log \int_{\mathbb{R}} \omega_\lambda^N[\mathcal{Q}_j^N(\mathrm{d}z)]\, e^{\kappa z N} \\
&\equiv p(\lambda) + \lim_{N\uparrow+\infty} \frac{1}{N} \log \int_{\mathbb{R}} \nu_j^N(\mathrm{d}z)\, e^{\kappa z N}
\end{aligned} \tag{13.33}$$

where we have introduced the (classical) probability measures ν_j^N as the distribution of M_j^N under states ω_λ^N. Denote the last term as $\psi_j(\kappa)$, and fix some $\delta > 0$. One has the estimate

$$\int_{\mathbb{R}} \nu_j^N(\mathrm{d}z)\, e^{\kappa z N} \geq e^{\kappa(m_j+\delta)N} \nu_j^N[z \geq m_j + \delta] \tag{13.34}$$

which implies, by the existence of the limiting generating function,

$$\limsup_{N\uparrow+\infty} \frac{1}{N} \log \nu_j^N[z \geq m_j + \delta] \leq \psi_j(\kappa) - \kappa(m_j + \delta) \tag{13.35}$$

---

[26] $e^{A+B} \leq e^A e^B$ for all hermitian matrices A, B.

for all $0 \leq \kappa \leq \kappa_0$. Since $\frac{d\psi_j}{d\kappa}|_{\kappa=0} = m_j$, there exists $\kappa_1 = \kappa_1(\delta)$, $0 < \kappa_1 \leq \kappa_0$ such that $\psi_j(\kappa_1) \leq \kappa_1 m_j + \frac{\kappa_1 \delta}{2}$. Hence,

$$\limsup_{N\uparrow+\infty} \frac{1}{N} \log \nu_j^N[z \geq m_j + \delta] \leq -\frac{\kappa_1 \delta}{2} \tag{13.36}$$

Combining with an analogous argument for $\nu_j^N[z \leq m_j - \delta]$, we arrive at the bound

$$\omega_\lambda^N[Q_j^{N,\delta}(m_j)] \geq 1 - e^{-C_j(\delta)N} \tag{13.37}$$

valid for all $\delta > 0$ and $N \geq N_j(\delta)$, with some $C_j(\delta) > 0$ and $N_j(\delta)$; the $\mathcal{Q}_j^{N,\delta}(m_j)$ is given by (13.4).

   This in particular implies that states ω_λ^N are concentrating at $m(\lambda)$ in the sense of a law of large numbers analogous to (13.10); moreover, the concentration is exponentially fast. Note that the above argument is similar to the construction of large deviation upper bounds, cf. any textbook on the large deviation theory, e.g. [9, 23].

   In an analogous way we exploit assumption (1) on the pressure. This time we consider the observable $\sum_k \lambda_k M_k^N$ and denote by $\bar{\mathcal{Q}}^N$ the corresponding projection-valued measure, i.e., such that

$$F\left(\sum_k \lambda_k M_k^N\right) = \int_{\mathbb{R}} \bar{\mathcal{Q}}^N(dz)\, F(z), \qquad F \in C(\mathbb{R}) \tag{13.38}$$

Repeating the arguments (13.33)–(13.37), we get the result

$$\omega_\lambda^N[\bar{Q}^{N,\delta}] \geq 1 - e^{-\bar{C}(\delta)N} \tag{13.39}$$

with

$$\bar{Q}^{N,\delta} = \int_{\mathbb{R}} \bar{Q}^N(dz)\, \chi\left(\sum_k \lambda_k m_k - \delta \leq z \leq \sum_k \lambda_k m_k + \delta\right) \tag{13.40}$$

valid again for all $\delta > 0$, $N \geq \bar{N}(\delta)$, with some $\bar{C}(\delta) > 0$ and $\bar{N}(\delta)$.

13.4.2. *Typical projections.* From (13.39) there is a sequence $\delta_N \downarrow 0$ such that the projections $\mathcal{P}^N = \bar{\mathcal{Q}}^{N,\delta_N}$ satisfy

$$\lim_{N\uparrow+\infty} \omega_\lambda^N[\mathcal{P}^N] = 1 \tag{13.41}$$

By construction one has the operator inequalities

$$\mathcal{P}^N\left(\sum_k \lambda_k m_k - \delta_N\right) \leq \mathcal{P}^N \sum_k \lambda_k M_k^N \leq \mathcal{P}^N\left(\sum_k \lambda_k m_k + \delta_N\right) \tag{13.42}$$

which yield the upper bound

$$\text{Tr}^N[\mathcal{P}^N] = \omega_\lambda^N[(\rho_\lambda^N)^{-1}\mathcal{P}^N] \leq \mathcal{Z}_\lambda^N e^{-N\left(\sum_k \lambda_k m_k - \delta_N\right)} \omega_\lambda^N[\mathcal{P}^N] \tag{13.43}$$

and the lower bound

$$\text{Tr}^N[\mathcal{P}^N] \geq \mathcal{Z}_\lambda^N e^{-N\left(\sum_k \lambda_k m_k + \delta_N\right)} \omega_\lambda^N[\mathcal{P}^N] \tag{13.44}$$

Using (13.41) and (13.27), this proves[27]

$$\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[\mathcal{P}^N] = p(\lambda) - \sum_k \lambda_k m_k = s_{\mathrm{can}}(m) \qquad (13.45)$$

As soon as we prove that projections $\mathcal{P}^N$ are concentrating at m (see the next section), the last equation simply means that $s(m) \geq s_{\mathrm{can}}(m)$. Since the opposite inequality is obvious, we arrive at (13.31) as claimed.

The arguments used in this section are well known in both classical and quantum information theory, and projections $\mathcal{P}^N$ satisfying (13.41) and (13.45) are usually called *typical (sequence of) projections*. Their existence under mild assumptions for a large class of models is a subject of the Shannon-McMillan(-Breiman) theorem, see e.g. [3] and references therein. For a nice overview of the principles of quantum information theory see [8].

13.4.3. *Concentration of typical projections.* To finish the proof we need to show that $\mathcal{P}^N$ as constructed in the last section concentrate at m. The following is true for any $Y^N \geq 0$:

$$\begin{aligned}
\omega_\lambda^N[Y^N] &= \mathrm{Tr}^N[(\rho_\lambda^N)^{\frac{1}{2}} Y^N (\rho_\lambda^N)^{\frac{1}{2}}] \\
&\geq \mathrm{Tr}^N[\mathcal{P}^N (\rho_\lambda^N)^{\frac{1}{2}} Y^N (\rho_\lambda^N)^{\frac{1}{2}} \mathcal{P}^N] \\
&= \mathrm{Tr}^N[(Y^N)^{\frac{1}{2}} \mathcal{P}^N \rho_\lambda^N (Y^N)^{\frac{1}{2}}] \\
&\geq \frac{1}{\mathcal{Z}_\lambda^N} e^{N\left(\sum_k \lambda_k m_k - \delta_N\right)} \mathrm{Tr}^N[\mathcal{P}^N] \, \mathrm{tr}^N[Y^N \,|\, \mathcal{P}^N] \\
&\geq e^{-2N\delta_N} \omega^N[\mathcal{P}^N] \, \mathrm{tr}^N[Y^N \,|\, \mathcal{P}^N]
\end{aligned} \qquad (13.46)$$

where we have used inequalities (13.42) and (13.44). Take now $Y^N = 1 - \mathcal{Q}_j^{N,\epsilon}(m_j)$ and use the exponential concentration property of ω_λ^N, inequality (13.37); one obtains

$$1 - \mathrm{tr}^N[\mathcal{Q}_j^{N,\epsilon}(m_j) \,|\, \mathcal{P}^N] \leq e^{-(C_j(\epsilon) - 2\delta_N)N} (\omega_\lambda^N[\mathcal{P}^N])^{-1} \qquad (13.47)$$

for any $\epsilon > 0$ and $N \geq N_j(\epsilon)$, which immediately gives[28]

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N[\mathcal{Q}_j^{N,\epsilon}(m_j) \,|\, \mathcal{P}^N] = 1 \qquad (13.48)$$

Repeating for all $j \in I$, this proves $\mathcal{P}^N \to m$.

---

[27]Note that one only needs that $\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[\mathcal{P}^N] = 0$. In particular, the assumption on the differentiability of the pressure is convenient but far from necessary; see also a comment below.

[28]Note it actually yields an exponential concentration, even under that weaker assumption $\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N[\mathcal{P}^N] = 0$.

13.5. **Towards quantum large deviations.** Using the notation of Section 13.4.1, the Gärtner-Ellis theorem of (classical) large deviations, [9, 23], teaches us that whenever the generating function $q_j \in C^1(\mathbb{R})$ is differentiable and strictly convex, one has the law

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow \infty} \frac{1}{N} \log \nu_j^N [z \overset{\delta}{=} \tilde{m}_j] = -I_j(\tilde{m}_j) \tag{13.49}$$

for any $\tilde{m}_j$ such that $\tilde{m}_j = \frac{\mathrm{d}q_j}{\mathrm{d}\kappa}\big|_{\kappa = \kappa(\tilde{m}_j)}$ for some (unique by assumption) $\kappa(\tilde{m}_j)$, and with the rate function I_j being the Legendre transform

$$\begin{aligned} I_j(\tilde{m}_j) &= \sup_{\kappa}\Big\{ \kappa\, \tilde{m}_j - \lim_{N \uparrow +\infty} \frac{1}{N} \log \omega_\lambda^N \big[e^{\kappa N M_j^N} \big] \Big\} \\ &= \sup_{\kappa} [\kappa\, \tilde{m}_j - q_j(\kappa) + p(\lambda)] \\ &= \kappa(\tilde{m}_j)\, \tilde{m}_j - q_j(\kappa(\tilde{m}_j)) + p(\lambda) \end{aligned} \tag{13.50}$$

(Naturally, for m such that $\omega_\lambda^N \overset{1}{\to} m$ one has $\kappa(m_j) = 0$ and $I_j(m_j) = 0$.) In terms of the canonical states ω_λ^N, (13.49) becomes simply

$$\lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \omega_\lambda^N [\mathcal{Q}_j^{N,\delta}(\tilde{m}_j)] = -I_j(\tilde{m}_j) \tag{13.51}$$

This is an exponential law for the outcomes of measurements of the observables M_j^N, upon the canonical states ω_λ^N. This gives an interpretation to q_j as the corresponding generating function.

The existence and differentiability of q_j gets nontrivial whenever the observables M_k^N are more complicated than just something like the spatial averages of one-site observables over a lattice (a simple example are the observables M_1^N, M_2^N, M_3^N in the quantum Kac model, Section 14). In the usual context of quantum lattice models, no general argument is known even for the existence of $q_j(\kappa)$, which is in contrast to the case of pressure $p(\lambda)$ where the situation is rather well understood, [51, 24, 5]. For some partial results about the existence of q_j in the so called high-temperature regime see [45, 49]; the differentiability is studied in [45].

By means of the Varadhan lemma, [9], formula (13.51) can be equivalently written as

$$\lim_{N \uparrow +\infty} \frac{1}{N} \log \omega_\lambda^N [e^{NF(M_j^N)}] = \sup_z \{ F(z) - I_j(z) \} \tag{13.52}$$

for any $F \in C(\mathbb{R})$, for simplicity assumed to be bounded from above. This form provokes still another related question, namely the asymptotic limit

$$\lim_{N \uparrow +\infty} \frac{1}{N} \log \mathrm{Tr}^N [e^{N\left(\sum_k \lambda_k M_k^N + F(M_j^N) \right)}] \tag{13.53}$$

Although this is likely not directly related to the quantum fluctuations, such formulas appear naturally when studying lattice models with a combination of short-range and long-range interactions. Some authors

consider *this* formulation as a genuine problem of quantum large deviations; see e.g. [47] where the authors show the above limit to exist in the case of M_k^N being averages over one-site spin observables.[29] They prove the following variational principle:

$$(13.53) = \sup_z \{F(z) - I_j'(z)\}, \qquad I_j'(z) = \sup_\kappa \{\kappa\, z - q_j'(\kappa)\} \quad (13.54)$$

$$q_j'(\kappa) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \operatorname{Tr}^N\left[e^{N\left(\sum_k \lambda_k M_k^N + \kappa M_j^N\right)}\right] \qquad (13.55)$$

which is similar to (13.49)–(13.50) up to the modified generating function q'.

A general and systematic quantum large deviation theory is lacking, however, and remains an interesting open question. Possibly even more ambitious, both physically and mathematically, would be the problem of correlated large fluctuations for noncommuting macroscopic observables. Some ideas on this issue can be found in [2]; also the present construction of generalized microcanonical ensembles, Section 13.1.2, seems related to this problem.

14. EXAMPLE: QUANTUM KAC RING

This is a quantum extension of the Kac ring model of Section 10, introduced and studied in [15, 11]. Consider a ring $\Lambda = \{1,\ldots,N\}$ again, and associate with each site i a quantum spin $\eta(i) \in \mathbb{C}^2$ and a classical variable $g(i) \in \{1,0\}$ that indicates the presence respectively the absence of a scatterer. The state space of the model is hence $\mathcal{H}^N \times K^N$ with Hilbert space $\mathcal{H}^N = \mathbb{C}^{2N}$ (spins) and classical space $K^N = \{0,1\}^N$ (scatterers).

14.1. **Macroscopic description.** As macroscopic observables we consider the operators

$$M_\alpha^N = \frac{1}{N} \sum_{i=1}^N \sigma_\alpha(i), \qquad \alpha = 1,2,3 \qquad (14.1)$$

where $\sigma_\alpha(i)$ are copies at site i of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad (14.2)$$

representing three components of the local 'magnetization', and

$$M_0^N(g) = \frac{1}{N} \sum_{i=1}^N g(i) \qquad (14.3)$$

the density of scatterers. By construction, $[M_1^N, M_2^N] = \frac{1}{N} M_3^N$ (and cyclic permutations). The classical (= commutative) case is restored by keeping e.g. M_0^N and M_3^N as the only macroobservables.

---

[29] This in particular mean that the canonical states ω_λ^N are product states.

It is sometimes convenient to embed K^N in $\mathbb{C}^{2N}$ and to utilize a compact notation for both operators on $\mathcal{H}^N$ and classical functions on K^N. In this sense we speak below about states over $\mathcal{H}^N \times K^N$, and we use the shorthand $\hat{\mathrm{Tr}}^N = \sum_{g \in K^N} \mathrm{Tr}^N$.

In the canonical framework,

$$
\omega_\lambda^N(\cdot) = \frac{1}{\mathcal{Z}_\lambda^N} \hat{\mathrm{Tr}}^N[e^{N \sum_{\alpha=0}^3 \lambda_\alpha M_\alpha^N} \cdot]
$$

$$
= e^{-Np(\lambda)} \hat{\mathrm{Tr}}^N\left[e^{\sum_{i=1}^N \left(\lambda_0 g(i) + \sum_{\alpha=1}^3 \lambda_\alpha \sigma_\alpha(i)\right)} \cdot\right]
\tag{14.4}
$$

are product canonical states, and the pressure is

$$
p(\lambda) = \frac{1}{N} \log \hat{\mathrm{Tr}}^N[e^{N \sum_{\alpha=0}^3 \lambda_\alpha M_\alpha^N}] = \log 2[(1 + e^{\lambda_0}) \cosh |\vec{\lambda}|]
\tag{14.5}
$$

with the shorthands $\vec{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$ and $|\vec{\lambda}| = (\lambda_1^2 + \lambda_2^2 + \lambda_3^2)^{\frac{1}{2}}$. Further, $\omega_\lambda^N \xrightarrow{1} m$ where

$$
m_0 = \frac{\partial p}{\partial \lambda_0} = (1 + e^{-\lambda_0})^{-1}, \quad m_\alpha = \frac{\partial p}{\partial \lambda_\alpha} = \frac{\lambda_\alpha}{|\vec{\lambda}|} \tanh |\vec{\lambda}|, \ \alpha = 1, 2, 3
\tag{14.6}
$$

The canonical entropy is then, $m = (m_0, \vec{m})$,

$$
s_{\mathrm{can}}(m) = p(\lambda) - \sum_{\alpha=0}^3 \lambda_\alpha m_\alpha
$$

$$
= \begin{cases} -\frac{1+|\vec{m}|}{2} \log \frac{1+|\vec{m}|}{2} - \frac{1-|\vec{m}|}{2} \log \frac{1-|\vec{m}|}{2} \\ \quad -m_0 \log m_0 - (1 - m_0) \log(1 - m_0) & \text{if } |\vec{m}| < 1, \, 0 < m_0 < 1 \\ -\infty & \text{otherwise} \end{cases}
\tag{14.7}
$$

cf. the classical case, (10.11).

To obtain a microcanonical description in the sense of Section 13.1.2, we associate with any macroscopic state $m = (m_0, \vec{m})$ the *modified* macroscopic observable $(M_0^N, \bar{M}^N)$,

$$
\bar{M}^N = \sum_{\alpha=1}^3 \frac{m_\alpha}{|\vec{m}|} M_\alpha^N = \frac{1}{N} \sum_{i=1}^N \bar{\sigma}(i), \qquad \bar{\sigma} = \frac{\vec{m}}{|\vec{m}|} \cdot \vec{\sigma}
\tag{14.8}
$$

and the modified macrostate $(m_0, |\vec{m}|)$.

Since $\bar{\sigma}$ is unitarily equivalent to e.g. σ_3, i.e., $\bar{\sigma} = W \sigma_3 W^\dagger$ with some $W^\dagger = W^{-1}$, we are back at the classical (commutative) situation. Denoting by $\bar{\mathcal{Q}}^N(\mathrm{d}z)$ the projection-valued measure for $(M_0^N, \bar{M}^N)$, one easily checks that any[30] $\bar{\mathcal{Q}}^{N,\delta_N}(m_0, |\vec{m}|)$ such that $\delta_N \downarrow 0$, are concentrating projections at $(m_0, |\vec{m}|)$. Moreover, if $N^{\frac{1}{2}} \delta_N \uparrow +\infty$ then these

---

[30]The notation is the same as in Section 13.1.

are *typical* concentrating projections at $(m_0, |\vec{m}|)$ and the entropy is, as essentially can be read off from the classical formula (10.11),

$$s(m_0, |\vec{m}|) = \lim_{N \uparrow +\infty} \frac{1}{N} \log \hat{\mathrm{Tr}}^N [\bar{\mathcal{Q}}^{N, \delta_N}(m_0, |\vec{m}|)] = s_{\mathrm{can}}(m_0, \vec{m}) \quad (14.9)$$

In the last step, we need to show that $\bar{\mathcal{Q}}^{N, \delta_N}(m_0, |\vec{m}|)$ are also concentrating at $m = (m_0, \vec{m})$, that is the macrostate under the *original* (noncommuting family of) macroscopic observables M^N. This can be proven by essentially repeating the argument of Section 13.4.3; we leave it to reader as an exercise. As a result, those $\bar{\mathcal{Q}}^{N, \delta_N}(m_0, |\vec{m}|)$ are typical projections concentrating at $m = (m_0, \vec{m})$.

14.2. **Microscopic dynamics.** To model the scattering of quantum spins (represented by vector η) on the binary variable g, consider a unitary matrix V on $\mathbb{C}^2$,

$$V = e^{i\vec{h} \cdot \vec{\sigma}}, \qquad \vec{h} = (h_1, h_2, h_3) \quad (14.10)$$

Let the dynamics on $\mathcal{H}^N \times K^N$ be given as, cf. (10.1),

$$U^N(\eta; g) = \big(g(N) \, V\eta(N) + (1 - g(N)) \, \eta(N),$$
$$g(1) \, V\eta(1) + (1 - g(1)) \, \eta(1), \dots,$$
$$\dots, g(N-1) \, V\eta(N-1) + (1 - g(N-1)) \, \eta(N-1); \, g\big) \quad (14.11)$$

extended to a unitary operator in the quantum sector by linearity. The associated automorphisms are then

$$\tau_t^N(\cdot) = (U^N)^{-t} \cdot (U^N)^t \quad (14.12)$$

14.3. **Macroscopic dynamics.** Let us start with a heuristic argument in the spirit of Boltzmann's Stosszahlansatz. Any macrostate $m = (m_0, \vec{m})$ can be associated with the quantum state of a *single* 'effective' quantum spin, via the 2×2 density matrix

$$\nu = \frac{1}{2}(\mathbb{1} + \vec{m} \cdot \vec{\sigma}), \qquad \mathrm{Tr}[\nu \, \sigma_\alpha] = m_\alpha, \ \alpha = 1, 2, 3 \quad (14.13)$$

Each time step the effective spin either meets a scatterer (with probability m_0) or not (with probability $1 - m_0$). Hence, its evolution is presumably $\nu \mapsto \nu_t = \bar{\phi}^t(\nu)$,

$$\bar{\phi}(\nu) = m_0 V \nu V^\dagger + (1 - m_0) \, \nu \quad (14.14)$$

by construction enjoying the semigroup property. Using (14.10) and (14.13), this can be explicitly written as the evolution on macrostates: $m_{t+1} = \phi(m_t)$ where

$$\phi(m_0, \vec{m}) = (m_0, \ \vec{m} - 2m_0[(\vec{n} \times \vec{m}) \sin |\vec{h}| \cos |\vec{h}| - \vec{n} \times (\vec{n} \times \vec{m}) \sin^2 |\vec{h}|])$$
$$(14.15)$$

with the notation $\vec{n} = \vec{h}/|\vec{h}|$. One easily checks that $\vec{h} \cdot \vec{m}$ is invariant under ϕ; the evolution can be visualized as a spiral motion in the plane perpendicular to $\vec{n}$. Provided that $|\vec{h}| \neq 0, \pi, 2\pi, \ldots$ and $m_0 \in (0, 1)$,

$$\lim_{t \uparrow +\infty} \phi^t(m_0, \vec{m}) = (m_0, (\vec{n} \cdot \vec{m}) \, \vec{n}) \tag{14.16}$$

and the relaxation is exponentially fast. The monotonicity of the entropy $s(m_t)$ can also be easily verified.

A rigorous argument showing that the above heuristics is indeed correct was given in [10], employing a strategy similar to that for the classical Kac model, Section 10.2. The result reads that for a large class of (sequences of) states $\omega^N \xrightarrow{1} m$, including in particular

- the (microcanonical) states $\mathrm{tr}^N[\,\cdot\,|\,\bar{\mathcal{Q}}^{N,\delta_N}(m, |\vec{m}|)]$ under those typical concentrating projections at m constructed in Section 14.1;
- the canonical states ω_λ^N from (14.4);

one has the law of large numbers:

$$\omega^N[\tau_t^N F(M_\alpha^N)] = F((\phi_t m)_\alpha), \qquad \alpha = 1, 2, 3 \tag{14.17}$$

for all $F \in C(\mathbb{R})$ and with ϕ given by (14.15). Hence, one verifies the autonomy condition (13.15).

14.4. **Exercise.** Consider (M_0^N, M_3^N) as a new macroscopic observable. Check that the data (m_0, m_3) are macroscopically equivalent with $(m_0, 0, 0, m_3)$ for the original 'full' macroscopic observable M^N; therefore the autonomy just follows from (14.17). Calculate the entropy $s(m_0, m_3)$ and show that it oscillates as a function of time. How can this apparent failure of the H-theorem be explained?

15. Concluding remarks

The text has discussed some newer and some older issues of nonequilibrium physics. Main emphasis has been on fluctuations and on the relation between entropy and irreversibility. One could say that everything has been an exploration of the idea that entropy production is a measure of irreversibility. Some central identities have been (4.7), (7.5), (10.25) and (11.9) which all point to the deep connection between source terms of time-reversal breaking and statistical thermodynamic quantities. They go beyond standard irreversible thermodynamics because fluctuations play an essential role here. As known since long, the deviations of thermodynamic behavior are important in the very understanding of its microscopic origin. These relations go also beyond the standard schemes as they are not perturbative and they do not require linear approximations or closeness to equilibrium.

Nevertheless there is also a sense in which all that has been attempted here does remain very close to the standard perspective. We

do not mean only that there is not really much fundamentally new since Boltzmann's statistical interpretation of entropy. It is true that progress has been very slow and we have been writing mostly from the point of view of the rear-guard, dissecting arguments and explanations that have been won long before. What we do have in mind however is that the theory so far remains very much restricted to direct comparisons with equilibrium. The obsession with time has mostly been an interest in the passing away of structure, of deleting memory and of ending in equilibrium—all the time centering around the second law of thermodynamics, and often applying Markovian schemes or justifying molecular chaos. We hope that the lectures that are summarized in the preceding sections have indeed clarified some of these issues, but we do not want to leave the reader without trying to provoke some feeling of totally different directions.

The most sensational instances of nonequilibrium physics are probably not be found in the problem of relaxation to equilibrium nor in the installation of nonequilibrium via standard thermodynamic forces for which the linear response theory appears to be working well even quite far from equilibrium. What needs to be understood is the constructive role of fluctuations far away from equilibrium. For example, understanding nonequilibrium aspects in life processes be it for molecular motors or for the problem of protein folding, requires fundamental studies in reaction-rate theory. Ratchet mechanisms and the physics of transport and dissipation on very small scales must be part of it also. Nonequilibrium issues that are related to macroscopic structure (even on cosmic scales), to pattern formation and to the organization of robust steady behavior are mind-boggling, but one has to open them also via the methods and the traditions of mathematical statistical physics when one wants its role to go further than "simplification and reduction of the results of previous investigations to a form in which the mind can grasp them."[31]

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[31]J. C. Maxwell, in: *On Faraday's lines of forces.*

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